JAN 117638

U.S. DEPARTMENT OF COMMERCE
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SEARCH REQUEST FORM

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JAN

1-9

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- ✓ Structure
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USCOMM-DC 90-3952

PTO-1590 (9-90)

★ U.S. GPO: 1995-398-798/22489

STIC Search Report
Biotech-Chem Library

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TO:	From:
Ralph J Gitomer Location: 3d65 / 3e71 Saturday, March 27, 2004 Art Unit: 1651 Phone: 272-0916 Serial Number: 10 / 068333	Jan Delaval Location: Biotech-Chem Library Rem 1A51 Phone: 272-2504 jan.delaval@uspto.gov

3E71

Search Notes

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L2           142 S E3-E5,E12-E17
               E THEODORAKIS E/AU
L3            65 S E4-E8
L4             1 S L1 AND L2,L3
L5           199 S L2,L3 NOT L4
               SEL RN L4

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L8            50 S L6 NOT L7

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L14           66 S L8,L13
L15            0 S L14 NOT 2404.11/RID
L16            5 S L14 NOT 2404.11.33/RID
               E 2404.11.33/RID
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L19           66 S L14,L18
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L43          13 S L37 AND (PHARMACEUT? OR PHARMACOL?)/SC,SX
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L45           0 S (L30 OR L20)(L)FFD/RL
L46           0 S (L30 OR L20)(L)AGR/RL
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L49          20 S L47,L48
L50          24 S L36,L49
                SEL HIT RN

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FILE LAST UPDATED: 26 Mar 2004  (20040326/ED)

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=> d l50 all hitstr tot

L50  ANSWER 1 OF 24  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:689644  HCAPLUS
DN   139:381626
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ED Entered STN: 04 Sep 2003

TI Synthesis of a novel family of diterpenes and their evaluation as anti-inflammatory agents

AU Lam, Thanh; Ling, Taotao; Chowdhury, Chinmay; Chao, Ta-Hsiang; Bahjat, F. R.; Lloyd, G. K.; Moldawer, Lyle L.; **Palladino, Michael A.**; **Theodorakis, Emmanuel A.**

CS Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA, 92093-0358, USA

SO Bioorganic & Medicinal Chemistry Letters (2003), 13(19), 3217-3221
CODEN: BMCLE8; ISSN: 0960-894X

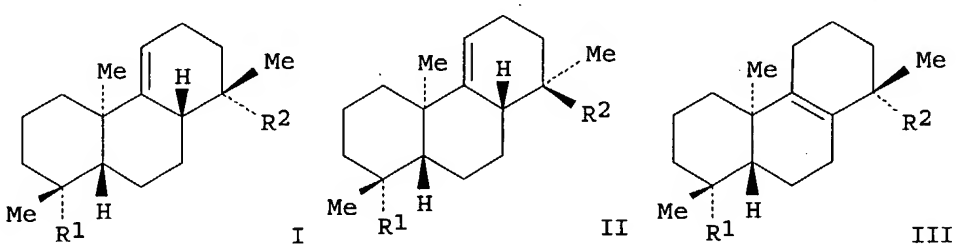
PB Elsevier Science B.V.

DT Journal

LA English

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1

GI



AB The synthesis and biol. evaluation of a new family of diterpenes, represented by structures I, II and III [R1 = CH2OH, CH:CH2; R2 = CO2Me, CH2OH, CO2H], is presented. These compds. constitute isomeric analogs of acanthoic acid and were examined as potent anti-inflammatory agents. Among them, Me ester I (R1 = CH:CH2; R2 = CO2Me) exhibited a low non-specific cytotoxicity, inhibited TNF-α synthesis and displayed good specificity in suppressing cytokine expression.

ST diterpene acanthoic acid isomeric analog prepn antiinflammatory cytotoxicity

IT Cytotoxicity
(of isomeric analogs of acanthoic acid against human peripheral blood mononuclear cells (HPBMC))

IT Human
Mononuclear cell (leukocyte)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity against human peripheral blood mononuclear cells (HPBMC))

IT Anti-inflammatory agents
Asymmetric synthesis and induction
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT Cytokines
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(selectivity of Me ester analogs of acanthoic acid)

IT Diterpenes
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(tricyclic; preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT 514-10-3, Abietic acid 5947-49-9, Podocarpic acid 66575-29-9,

Forskolin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(cytotoxicity and TNF-α inhibition)

IT **287401-13-2P 308795-78-0P** 467222-10-2P
467222-28-2P 467222-38-4P **623531-87-3P**
623531-88-4P
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT **308795-79-1P** 467222-37-3P **623531-89-5P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT 78-85-3, Methacrolein 1826-67-1, Vinylmagnesium bromide 187750-47-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT 287401-11-0P **308795-77-9P 467222-23-7P**
467222-24-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

IT **119290-87-8DP**, Acanthoic acid, isomeric analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

(1) Aggarwal, B; Human Cytokines: Their Role in Disease and Therapy 1995
(2) Ahmed, S; J Immunol Meth 1994, V170, P211 MEDLINE
(3) Allison, A; Ann N Y Acad Sci 1995, V762, P331 HCAPLUS
(4) Anon; Tumor Necrosis Factors. The Molecules and their Emerging Role in Medicine 1992
(5) Armstrong, A; Brit J Surg 1997, V84, P1051 MEDLINE
(6) Bathon, J; New Engl J Med 2000, V343, P1586 HCAPLUS
(7) Bauditz, J; New Engl J Med 1998, V338, P334 MEDLINE
(8) Camussi, G; Drugs 1998, V55, P613 HCAPLUS
(9) Camussi, G; Drugs 1998, V55, P613 HCAPLUS
(10) Dinarello, C; JAMA 1993, V269, P1829 MEDLINE
(11) Dinarello, C; Proinflammatory and Anti-inflammatory Cytokines in Rheumatoid Arthritis, 3rd ed 2001
(12) Ferrari, R; Cardiovasc Res 1998, V37, P554 HCAPLUS
(13) Firestein, G; Immunol 1990, V144, P3347 HCAPLUS
(14) Galvani, D; Cytokine Therapy 1992
(15) Hamilton, K; Expert Opin Pharmacother 2000, V5, P1041
(16) Hawkey, C; New Engl J Med 1998, V338, P333 MEDLINE
(17) Kang, H; Cell Immunol 1996, V170, P212 HCAPLUS
(18) Kang, H; Mediators Inflamm 1998, V7, P257 HCAPLUS
(19) Kim, Y; J Nat Prod 1988, V51, P1080 HCAPLUS
(20) Kurzrock, R; Cytokines: Interleukins and Their Receptors 1995
(21) Ling, T; J Org Chem 2001, V66, P8843 HCAPLUS
(22) Ling, T; Org Lett 2000, V2, P2073 HCAPLUS
(23) Lipsky, P; New Engl J Med 2000, V343, P1594 HCAPLUS
(24) Lorenz, H; Curr Opin Invest Drugs 2000, V1, P188 HCAPLUS
(25) Newton, R; J Med Chem 1999, V42, P2295 HCAPLUS
(26) Olsen, N; Arthritis Rheum 1996, V39, P1102 HCAPLUS
(27) Rutault, K; J Biol Chem 2001, V276, P6666 HCAPLUS
(28) Saxne, T; Arthritis Rheum 1988, V31, P1041 MEDLINE
(29) Souriaou, C; Exp Opin Biol Ther 2003, V3, P305

(30) Suh, Y; Bioorg Med Chem Lett 2001, V11, P559 HCAPLUS
(31) Szekanecz, Z; Clin Pharmacol 1998, V12, P377 MEDLINE
(32) Thorpe, R; Cytokines 1998
(33) van Den Berg, W; Arthritis Res 2001, V3, P18 HCAPLUS

IT **287401-13-2P 308795-78-0P 467222-28-2P 623531-87-3P 623531-88-4P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)

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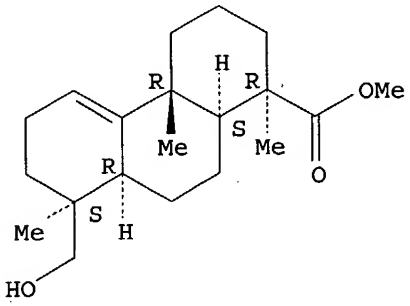
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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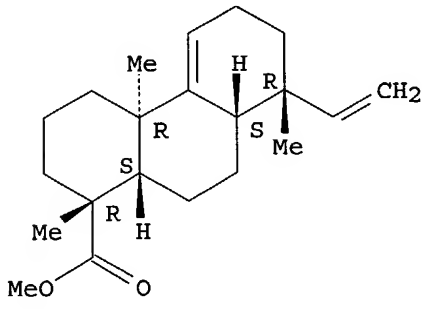
Absolute stereochemistry.



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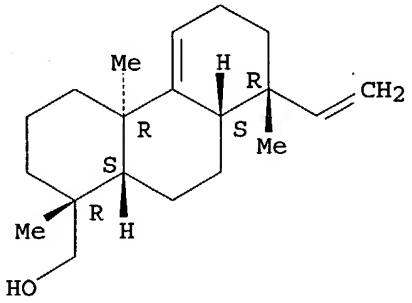
Absolute stereochemistry. Rotation (+).



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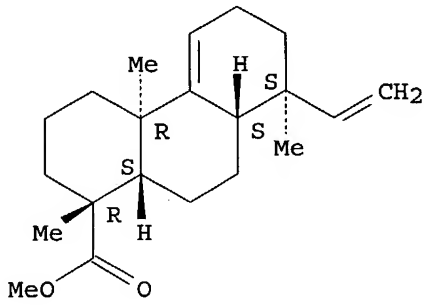
Absolute stereochemistry.



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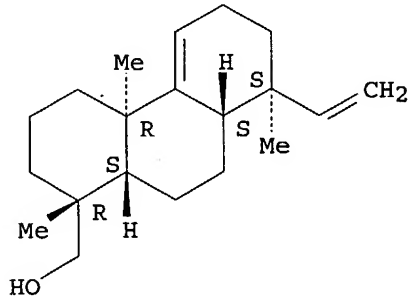
Absolute stereochemistry.



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RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)
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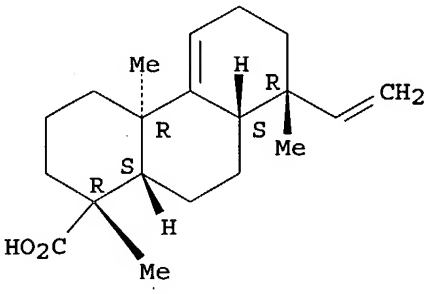
Absolute stereochemistry.



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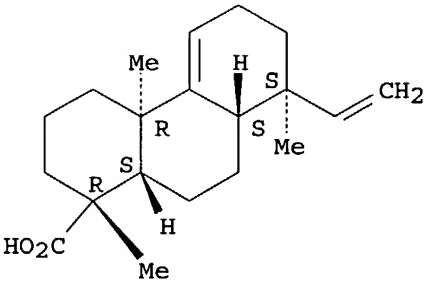
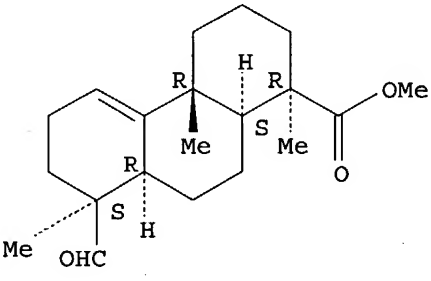
Absolute stereochemistry.



IT **308795-77-9P 467222-23-7P 467222-24-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)
RN 308795-77-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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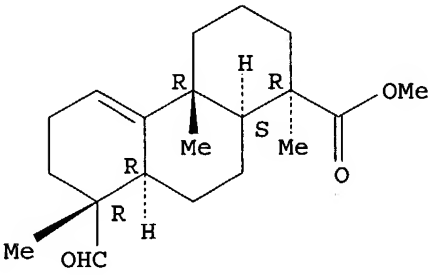
Absolute stereochemistry.



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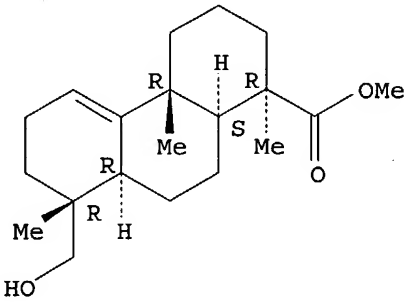
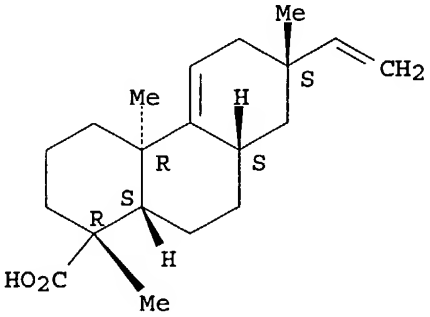
Absolute stereochemistry.



IT **119290-87-8DP**, Acanthoic acid, isomeric analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isomeric analogs of acanthoic acid and their evaluation for cytotoxicity and TNF-α inhibition)
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:203411 HCAPLUS
DN 138:238317
ED Entered STN: 14 Mar 2003
TI Preparation of interleukin-1 and tumor necrosis factor-α modulators

and their enantiomers

IN **Palladino, Michael; Theodorakis, Emmanuel A.**
PA USA

SO U.S. Pat. Appl. Publ., 77 pp., Cont.-in-part of U.S. Ser. No. 68,333.
CODEN: USXXCO
DT **Patent**
LA English
IC ICM A61K031-21
ICS A61K031-195; A61K031-19; A61K031-16; A61K031-13; A61K031-12
NCL 514529000; 514557000; 514623000; 514662000; 514691000; 560117000; 560005000; 562403000; 564188000; 564459000
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): **1**, **63**

FAN.CNT 3

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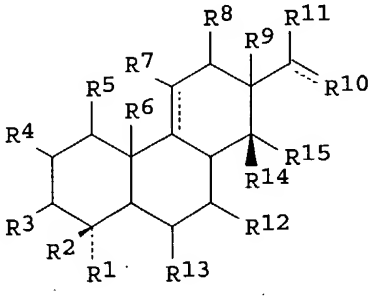

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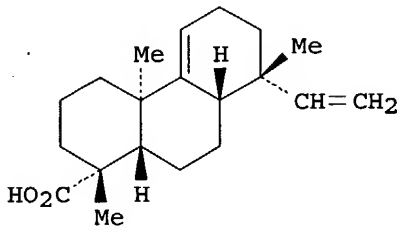


II

AB Novel compds. of formula I [R1 = H, halo, CO2H, alkyl-CO2H, acyl halide, etc.; R2, R9 = H, halo, alkyl, alkenyl, acyl, etc.; R3-R5, R7, R8, R11-R13 = H, halo, alkyl, aryl, etc.; R6 = H, halo, alkyl, alkenyl, alkynyl; R10 = H, halo, CH2, alkyl, aryl, etc.; R14, R15 = H, halo, alkyl, alkenyl, aryl, etc.] are prepared that are useful as interleukin-1 and tumor necrosis factor-α (TNF-α) modulators, and thus are useful in the treatment of various diseases. Pharmaceutical compns. comprising, and uses of, therapeutically effective amts. of the above compds. and their prodrug esters, and a pharmaceutically acceptable carrier, are also disclosed, and are useful as, for example, anti-inflammatory analgesics, in treating immune disorders, as anticancer and antitumor agents, and in the treatment of cardiovascular disease, skin redness, and viral infection. Completely synthetic and semi-synthetic methods of making these compds. and their analogs, are also disclosed. Thus, II was prepared from Wieland-Miescher ketone and methacrolein in several steps including a Diels-Alder reaction. II was shown to inhibit TNF-α production in a

human acute monocytic leukemia cell line.
ST interleukin 1 modulator prepn; tumor necrosis factor alpha modulator prepn
IT Eye, disease
Graves' disease
(Graves' ophthalmopathy; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Disease, animal
(Vogt-Koyanagi-Harada's syndrome; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Mouth, disease
(aphthous stomatitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Thyroid gland, disease
(autoimmune thyroiditis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Immunity
(disorder; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Transplant and Transplantation
(graft-vs.-host reaction; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(herpetic keratitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(infection; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(keratitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Glaucoma (disease)
(neovascular; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Goiter
(nodular; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Anti-inflammatory agents
(nonsteroidal; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Nerve, disease
(optic, neuritis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(periretinal proliferation; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Coagulation
(photocoagulation; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Pleura, disease
(pleurisy; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Allergy
Antitumor agents
Autoimmune disease
Behcet's syndrome
Cardiovascular system, disease
Diabetes mellitus
Eye, disease
Human
Inflammation
Ischemia
Multiple sclerosis
Neoplasm

Rabies
Skin, disease
Transplant rejection
Tuberculosis
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Interleukin 1
Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(retina, degeneration; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(retina, detachment; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(retinopathy; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Rheumatic diseases
(rheumatoid disease; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Connective tissue, disease
(scleroderma; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Shock (circulatory collapse)
(septic; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Respiratory tract, disease
(sinusitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(trachoma; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(uveitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Blood vessel, disease
(vasculitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Infection
(viral; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT **287401-13-2P 308795-78-0P 308795-79-1P**
RL: **PAC (Pharmacological activity)**; RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT **60855-32-5P 119290-87-8P**, NP 1302 **467221-99-4P**
467222-00-0P 467222-01-1P 467222-03-3P
467222-04-4P 467222-05-5P 467222-06-6P
467222-07-7P, LT 1-46 **467222-08-8P**, CC 3-13
467222-09-9P, CC 3-15 467222-10-2P **467222-11-3P**
467222-12-4P 467222-13-5P 467222-14-6P
467222-15-7P 467222-16-8P 467222-17-9P
467222-18-0P 467222-19-1P 467222-20-4P
467222-21-5P 467222-22-6P 501118-70-3P
RL: **PAC (Pharmacological activity)**; SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT 78-85-3, Methacrolein 78-94-4, Methyl vinyl ketone, reactions
107-10-8, n-Propylamine, reactions 108-30-5, Succinic anhydride, reactions 108-55-4, Glutaric anhydride 108-98-5, Thiophenol, reactions

109-01-3, N-Methyl piperazine 110-85-0, Piperazine, reactions
110-91-8, Morpholine, reactions 111-42-2, Diethanolamine, reactions
623-47-2, Ethyl propiolate 867-13-0, Triethyl phosphonoacetate
1193-55-1, 2-Methyl-1,3-cyclohexanedione 2605-67-6, Methyl (triphenylphosphoranylidene)acetate 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

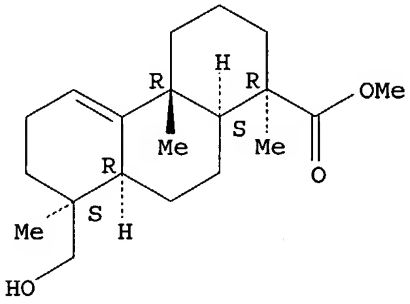
IT 5073-65-4P 100348-93-4P, (-)-Wieland-Miescher ketone
103462-23-3P 117556-90-8P 187750-47-6P 287401-06-3P
287401-07-4P 287401-08-5P 287401-09-6P 287401-11-0P 308795-75-7P
308795-76-8P **308795-77-9P 308795-83-7P**
467222-23-7P 467222-24-8P 467222-25-9P
467222-26-0P 467222-28-2P 467222-29-3P
467222-30-6P 467222-31-7P 467222-32-8P
467222-33-9P 467222-34-0P 467222-35-1P
467222-36-2P 467222-37-3P 467222-38-4P **467222-39-5P**
467222-40-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT **287401-15-4P 467222-27-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT **287401-13-2P 308795-78-0P 308795-79-1P**
RL: **PAC (Pharmacological activity)**; RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

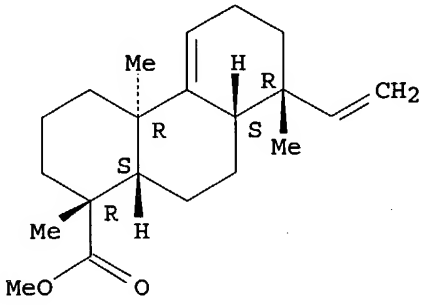
RN 287401-13-2 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



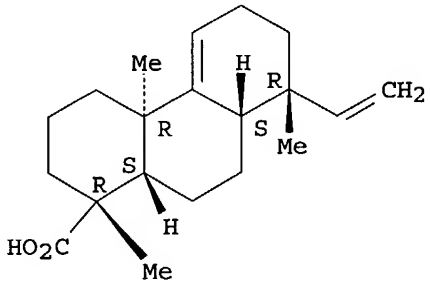
RN 308795-78-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



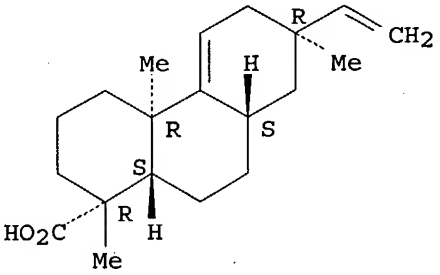
RN 308795-79-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



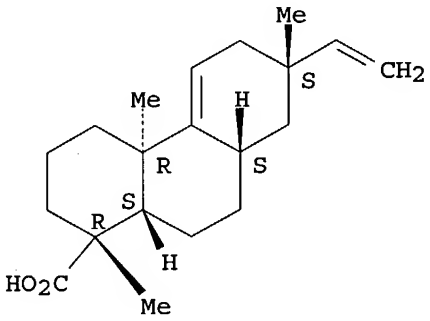
IT **60855-32-5P 119290-87-8P**, NP 1302 **467221-99-4P**
467222-00-0P 467222-01-1P 467222-03-3P
467222-04-4P 467222-05-5P 467222-06-6P
467222-07-7P, LT 1-46 **467222-08-8P**, CC 3-13
467222-09-9P, CC 3-15 **467222-11-3P 467222-12-4P**
467222-13-5P 467222-14-6P 467222-15-7P
467222-16-8P 467222-17-9P 467222-18-0P
467222-19-1P 467222-20-4P 467222-21-5P
467222-22-6P 501118-70-3P
RL: **PAC (Pharmacological activity)**; SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
RN 60855-32-5 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



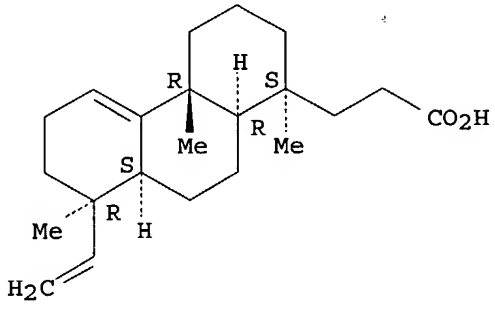
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



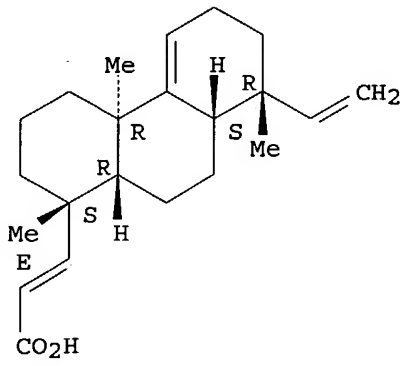
RN 467221-99-4 HCAPLUS
CN 1-Phenanthrenepropanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



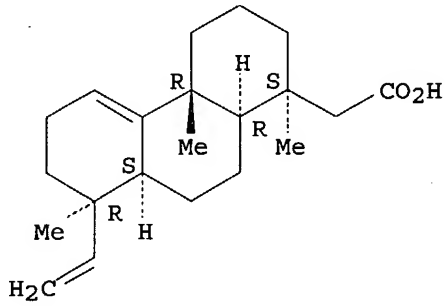
RN 467222-00-0 HCAPLUS
CN 2-Propenoic acid, 3-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



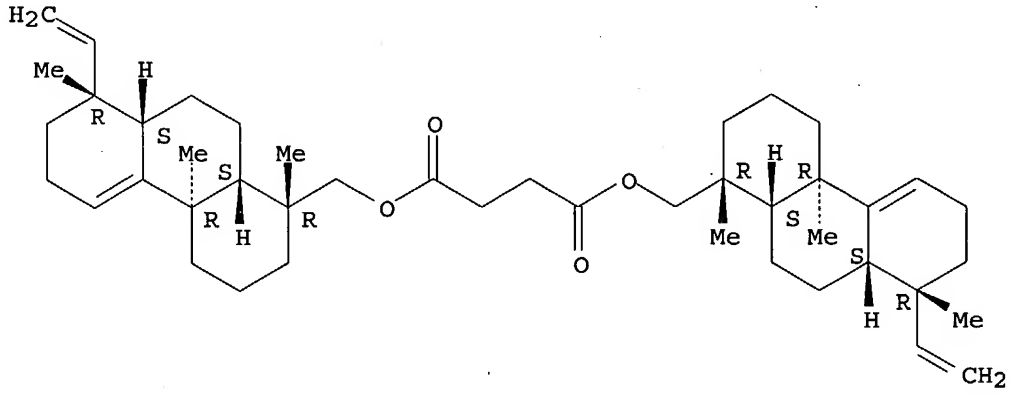
RN 467222-01-1 HCAPLUS
CN 1-Phenanthreneacetic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



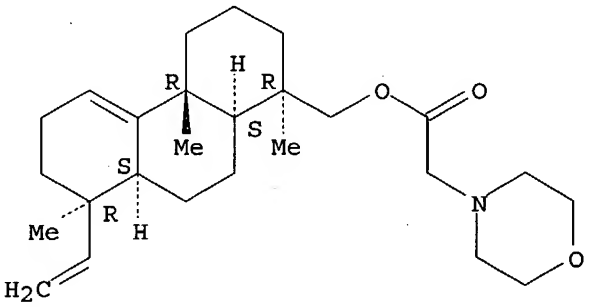
RN 467222-03-3 HCAPLUS
CN Butanedioic acid, bis[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



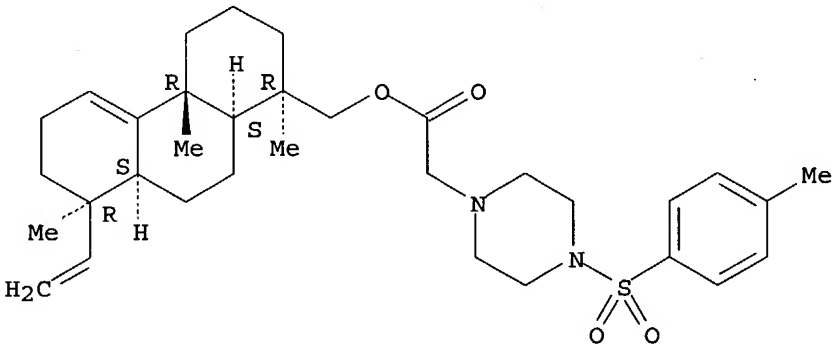
RN 467222-04-4 HCAPLUS
CN 4-Morpholineacetic acid, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



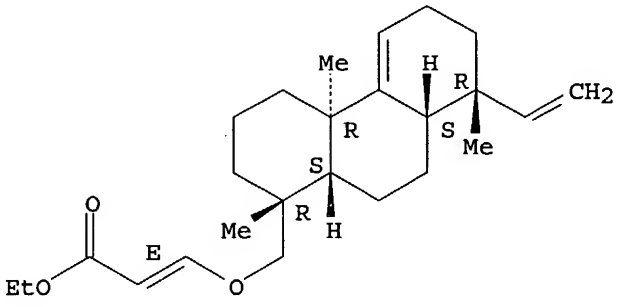
RN 467222-05-5 HCAPLUS
CN 1-Piperazineacetic acid, 4-[(4-methylphenyl)sulfonyl]-, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



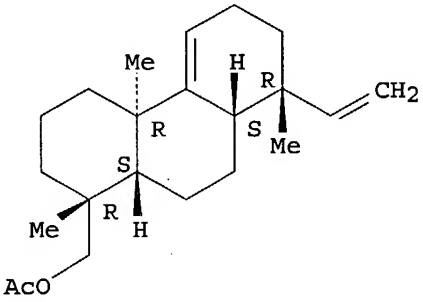
RN 467222-06-6 HCAPLUS
CN 2-Propenoic acid, 3-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methoxy]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



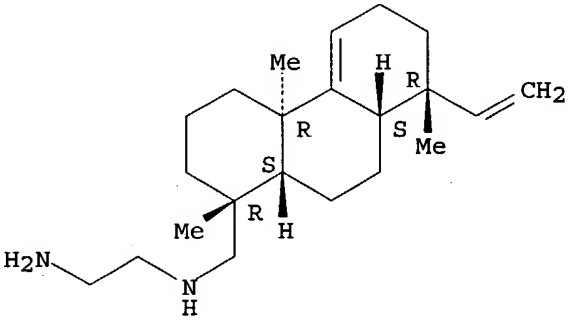
RN 467222-07-7 HCAPLUS
CN 1-Phenanthrenemethanol, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, acetate, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



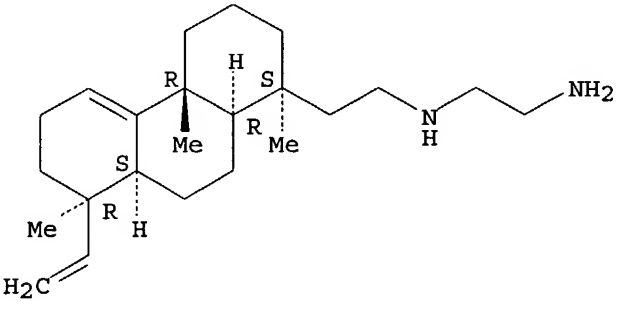
RN 467222-08-8 HCAPLUS
CN 1,2-Ethanediamine, N-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



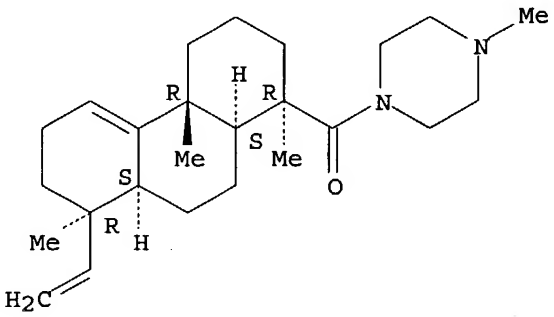
RN 467222-09-9 HCAPLUS
CN 1,2-Ethanediamine, N-[2-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



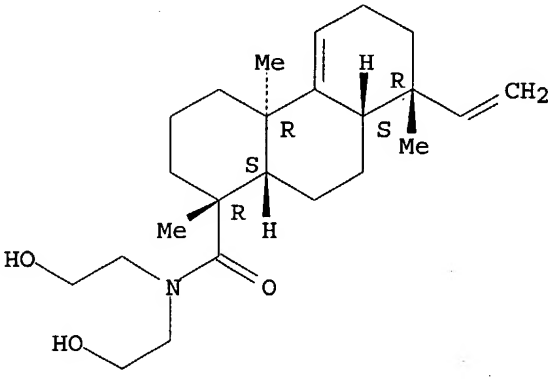
RN 467222-11-3 HCAPLUS
CN Piperazine, 1-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



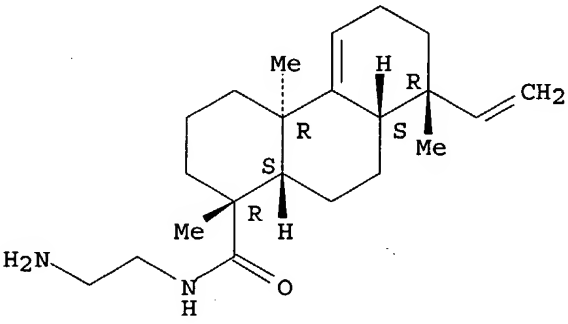
RN 467222-12-4 HCAPLUS
CN 1-Phenanthrenecarboxamide, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-N,N-bis(2-hydroxyethyl)-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



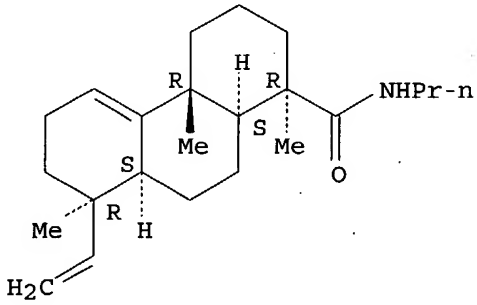
RN 467222-13-5 HCAPLUS
CN 1-Phenanthrenecarboxamide, N-(2-aminoethyl)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



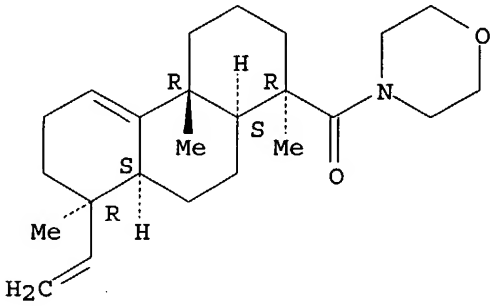
RN 467222-14-6 HCAPLUS
CN 1-Phenanthrenecarboxamide, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-N-propyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



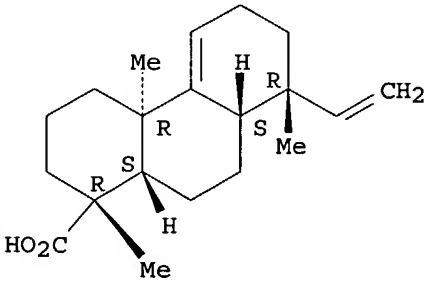
RN 467222-15-7 HCAPLUS
CN Morpholine, 4-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 467222-16-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, potassium salt, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

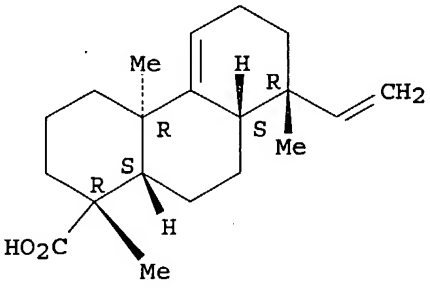
Absolute stereochemistry.



● K

RN 467222-17-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, sodium salt, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



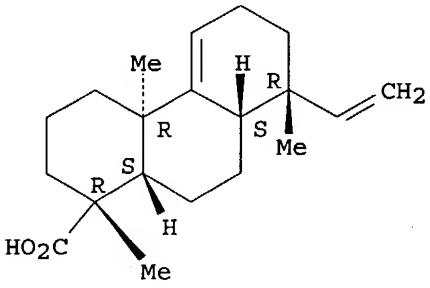
● Na

RN 467222-18-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)-, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (9CI) (CA INDEX NAME)

CM 1

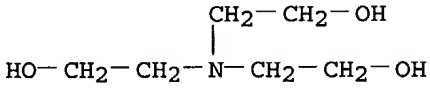
CRN 308795-79-1
CMF C20 H30 O2

Absolute stereochemistry.



CM 2

CRN 102-71-6
CMF C6 H15 N O3

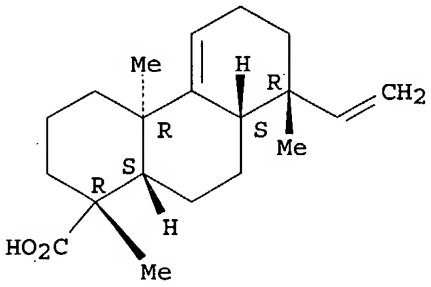


RN 467222-19-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)-, compd. with 2,2'-iminobis[ethanol] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 308795-79-1
CMF C20 H30 O2

Absolute stereochemistry.

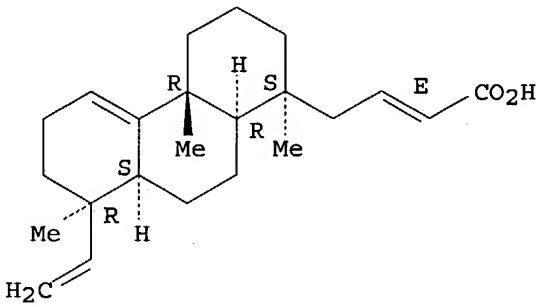


CM 2

CRN 111-42-2
CMF C4 H11 N O2

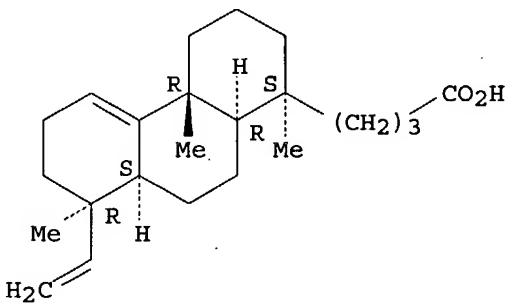
RN 467222-20-4 HCAPLUS
CN 2-Butenoic acid, 4-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



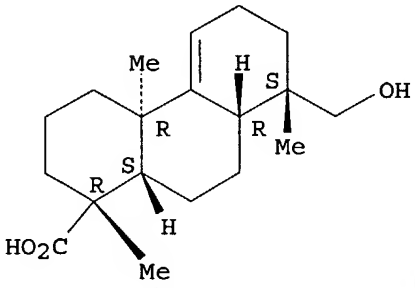
RN 467222-21-5 HCAPLUS
CN 1-Phenanthrenebutanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



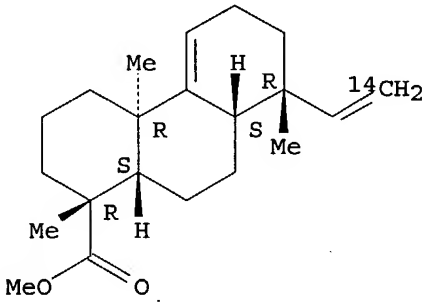
RN 467222-22-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



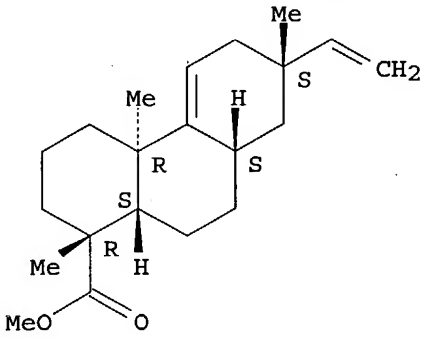
RN 501118-70-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-(ethenyl-2-14C)-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



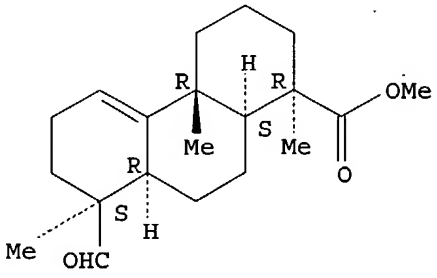
IT **103462-23-3P 308795-77-9P 308795-83-7P**
467222-23-7P 467222-24-8P 467222-26-0P
467222-28-2P 467222-29-3P 467222-30-6P
467222-31-7P 467222-32-8P 467222-33-9P
467222-34-0P 467222-35-1P 467222-36-2P
467222-39-5P 467222-40-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
RN 103462-23-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



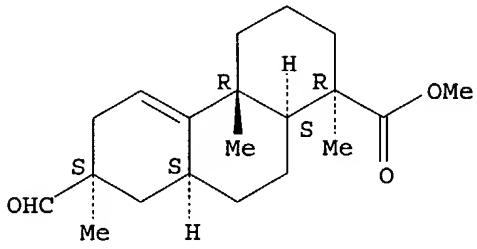
RN 308795-77-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



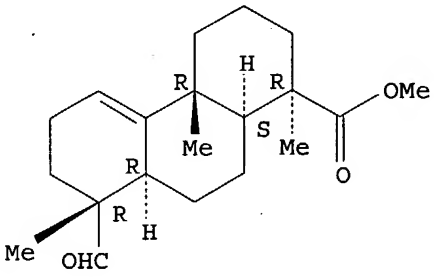
RN 308795-83-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



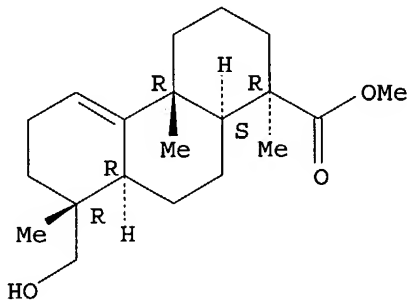
RN 467222-23-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



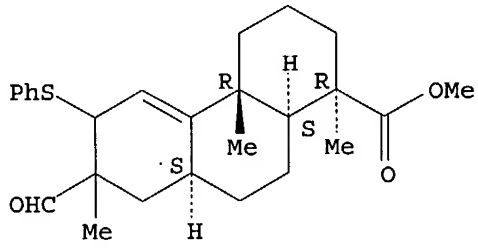
RN 467222-24-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



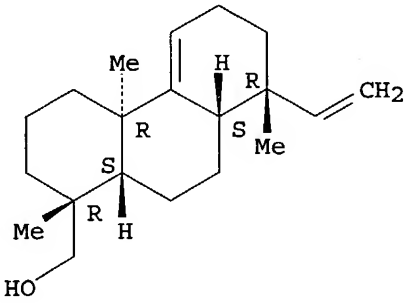
RN 467222-26-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-6-(phenylthio)-, methyl ester, (1R,4aR,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



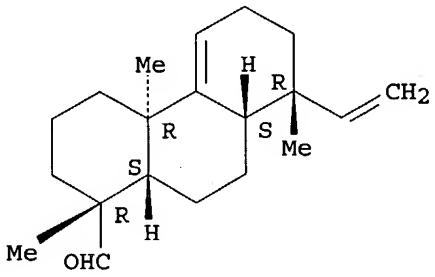
RN 467222-28-2 HCAPLUS
CN 1-Phenanthrenemethanol, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



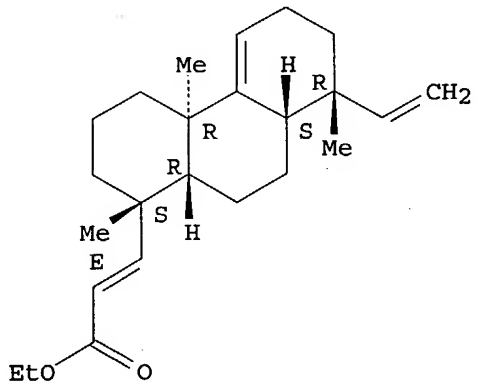
RN 467222-29-3 HCAPLUS
CN 1-Phenanthrenecarboxaldehyde, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



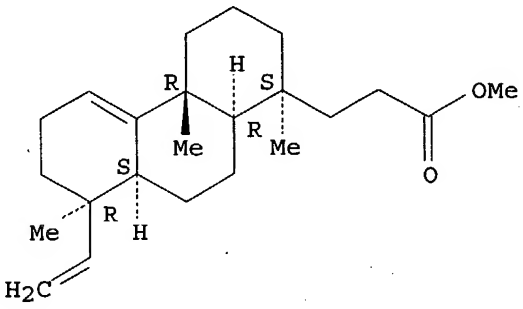
RN 467222-30-6 HCAPLUS
CN 2-Propenoic acid, 3-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



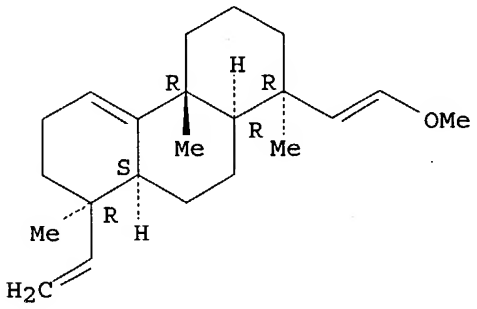
RN 467222-31-7 HCAPLUS
CN 1-Phenanthrenepropanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



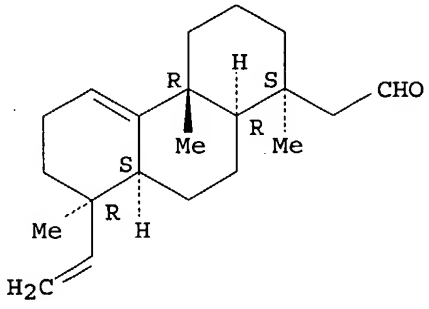
RN 467222-32-8 HCAPLUS
CN Phenanthrene, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1-(2-methoxyethenyl)-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



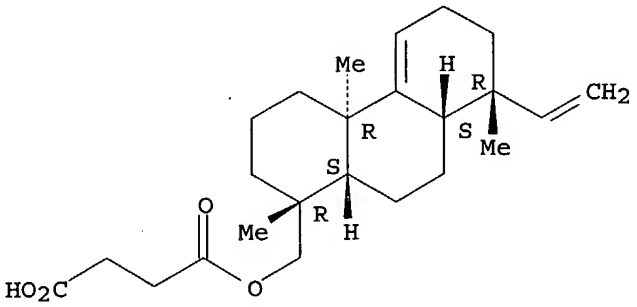
RN 467222-33-9 HCAPLUS
CN 1-Phenanthreneacetaldehyde, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



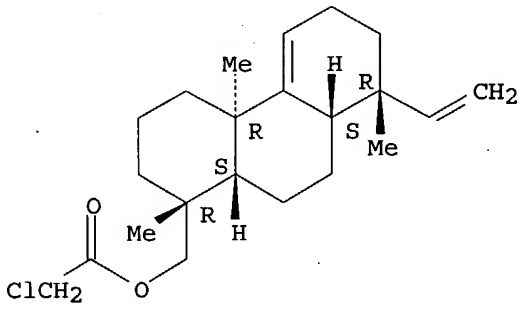
RN 467222-34-0 HCAPLUS
CN Butanedioic acid, mono[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



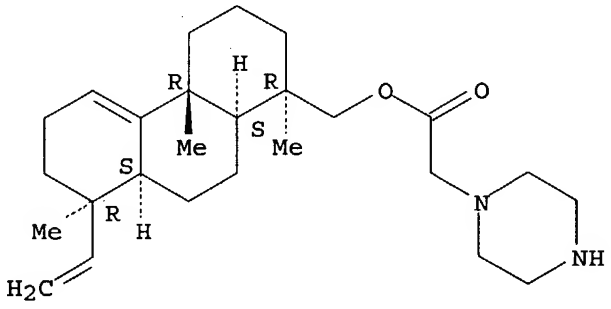
RN 467222-35-1 HCAPLUS
CN Acetic acid, chloro-, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



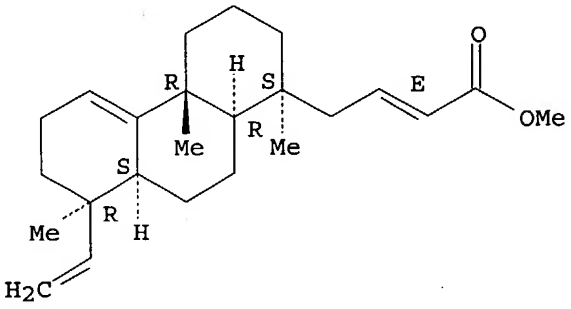
RN 467222-36-2 HCAPLUS
CN 1-Piperazineacetic acid, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



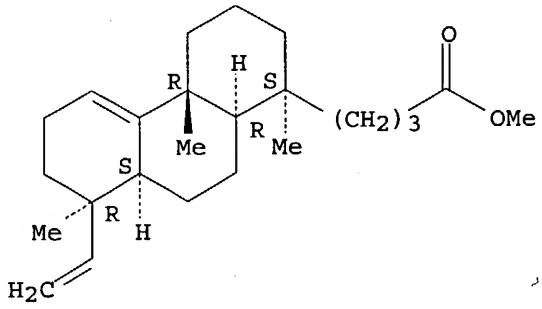
RN 467222-39-5 HCAPLUS
CN 2-Butenoic acid, 4-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



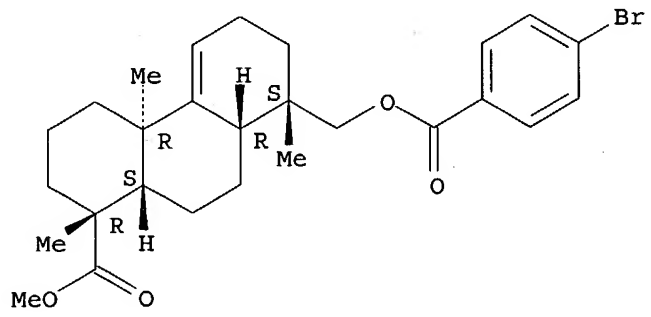
RN 467222-40-8 HCAPLUS
CN 1-Phenanthrenebutanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



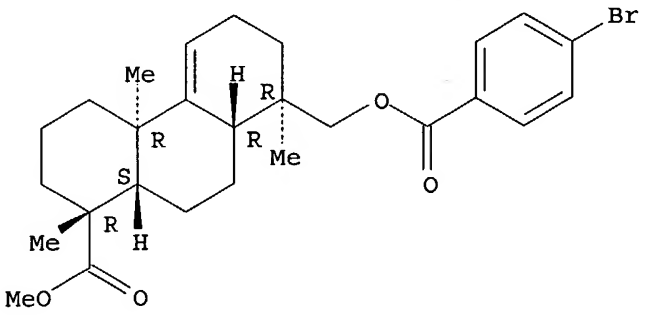
IT **287401-15-4P 467222-27-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
RN 287401-15-4 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 467222-27-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:777877 HCAPLUS
DN 137:279341
ED Entered STN: 11 Oct 2002
TI Preparation of interleukin-1 and tumor necrosis factor-α modulators and their enantiomers
IN **Palladino, Michael; Theodorakis, Emmanuel**
PA Nereus Pharmaceuticals, Inc., USA; The Regents of the University of California
SO PCT Int. Appl., 136 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C061-35
ICS C07C061-29; C07C069-753; C07C069-757; C07D295-185; C07C233-58; C07C233-62; C07C233-60; C07C033-14; C07C069-38; A61P037-02; A61K031-19; A61K031-215
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1, 63
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002079137	A1	20021010	WO 2002-US9591	20020327
WO 2002079137	C1	20021107		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2001-279381P P 20010328
US 2001-279952P P 20010329
US 2001-332031P P 20011121
OS MARPAT 137:279341
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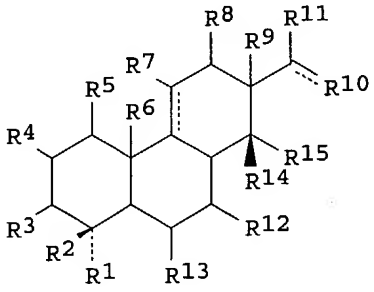

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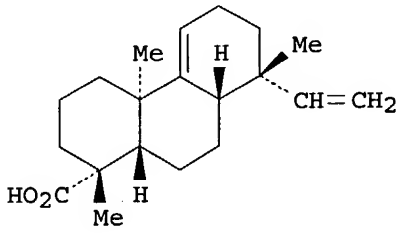


II

AB Novel compds. of formula I [R1 = H, halo, CO2H, alkyl-CO2H, acyl halide, etc.; R2, R9 = H, halo, alkyl, alkenyl, acyl, etc.; R3-R5, R7, R8, R11-R13 = H, halo, alkyl, aryl, etc.; R6 = H, halo, alkyl, alkenyl, alkynyl; R10 = H, halo, CH2, alkyl, aryl, etc.; R14, R15 = H, halo, alkyl, alkenyl, aryl, etc.] are prepared that are useful as interleukin-1 and tumor necrosis factor-α (TNF-α) modulators, and thus are useful in the treatment of various diseases. Pharmaceutical compns. comprising, and uses of, therapeutically effective amts. of the above compds. and their prodrug esters, and a pharmaceutically acceptable carrier, are also disclosed, and are useful as, for example, anti-inflammatory analgesics, in treating immune disorders, as anticancer and antitumor agents, and in the treatment of cardiovascular disease, skin redness, and viral infection. Completely synthetic and semi-synthetic methods of making these compds. and their analogs, are also disclosed. Thus, II was prepared from Wieland-Miescher ketone and methacrolein in several steps including a Diels-Alder reaction. II was shown to inhibit TNF-α production in a human acute monocytic leukemia cell line.

ST interleukin 1 modulator prepn; tumor necrosis factor alpha modulator prepn

IT Eye, disease
Graves' disease
(Graves' ophthalmopathy; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Disease, animal
(Vogt-Koyanagi-Harada's syndrome; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Mouth, disease
(aphthous stomatitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Thyroid gland, disease
(autoimmune thyroiditis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Immunity
(disorder; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Transplant and Transplantation
(graft-vs.-host reaction; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(herpetic keratitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(infection; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Eye, disease
(keratitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Glaucoma (disease)
(neovascular; preparation of interleukin-1 and tumor necrosis factor-α modulators)

IT Goiter
(nodular; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Anti-inflammatory agents
(nonsteroidal; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Nerve, disease
(optic, neuritis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(periretinal proliferation; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Coagulation
(photocoagulation; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Pleura, disease
(pleurisy; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Allergy
Antitumor agents
Autoimmune disease
Behcet's syndrome
Cardiovascular system, disease
Diabetes mellitus
Eye, disease
Human
Inflammation
Ischemia
Multiple sclerosis
Neoplasm
Rabies
Skin, disease
Transplant rejection
Tuberculosis
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Interleukin 1
Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(retina, degeneration; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(retina, detachment; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(retinopathy; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Rheumatic diseases
(rheumatoid disease; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Connective tissue, disease
(scleroderma; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Shock (circulatory collapse)
(septic; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Respiratory tract, disease
(sinusitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Eye, disease
(trachoma; preparation of interleukin-1 and tumor necrosis factor-α modulators)

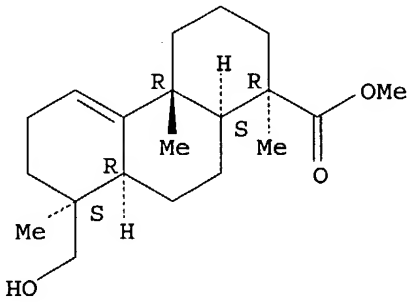
IT Eye, disease
(uveitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Blood vessel, disease
(vasculitis; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT Infection
(viral; preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT **287401-13-2P 308795-78-0P 308795-79-1P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT **60855-32-5P 119290-87-8P**, (-)-Acanthoic acid
467221-99-4P 467222-00-0P 467222-01-1P
467222-02-2P 467222-03-3P 467222-04-4P
467222-05-5P 467222-06-6P 467222-07-7P
467222-08-8P 467222-09-9P 467222-10-2P
467222-11-3P 467222-12-4P 467222-13-5P
467222-14-6P 467222-15-7P 467222-16-8P
467222-17-9P 467222-18-0P 467222-19-1P
467222-20-4P 467222-21-5P 467222-22-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT 78-85-3, Methacrolein 78-94-4, Methyl vinyl ketone, reactions
107-10-8, n-Propylamine, reactions 108-30-5, Succinic anhydride, reactions 108-55-4, Glutaric anhydride 108-98-5, Thiophenol, reactions
109-01-3, N-Methyl piperazine 110-85-0, Piperazine, reactions
110-91-8, Morpholine, reactions 111-42-2, Diethanolamine, reactions
623-47-2, Ethyl propiolate 867-13-0, Triethyl phosphonoacetate
1193-55-1, 2-Methyl-1,3-cyclohexanedione 2605-67-6, Methyl (triphenylphosphoranylidene)acetate 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT 5073-65-4P 100348-93-4P, (-)-Wieland-Miescher ketone
103462-23-3P 117556-90-8P 187750-47-6P 287401-06-3P
287401-07-4P 287401-08-5P 287401-09-6P 287401-11-0P 308795-75-7P
308795-76-8P **308795-77-9P 308795-83-7P**
467222-23-7P 467222-24-8P 467222-25-9P
467222-26-0P 467222-28-2P 467222-29-3P
467222-30-6P 467222-31-7P 467222-32-8P
467222-33-9P 467222-34-0P 467222-35-1P
467222-36-2P 467222-37-3P 467222-38-4P **467222-39-5P**
467222-40-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
IT **287401-15-4P 467222-27-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Kim, Y; JOURNAL OF NATURAL PRODUCTS 1988, V51(6), P1080 HCAPLUS
(2) Korea Inst Science Technology; WO 9534300 A 1995 HCAPLUS
(3) Lee, H; WO 9937600 A 1999 HCAPLUS
(4) Ling, T; ORGANIC LETTERS 2000, V2(14), P2073 HCAPLUS
(5) Suh, Y; BIOORGANIC & MEDICINAL CHEMISTRY LETTERS 2001, V11(4), P559 HCAPLUS
(6) Univ California; WO 0073253 A 2000 HCAPLUS
IT **287401-13-2P 308795-78-0P 308795-79-1P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

RN 287401-13-2 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

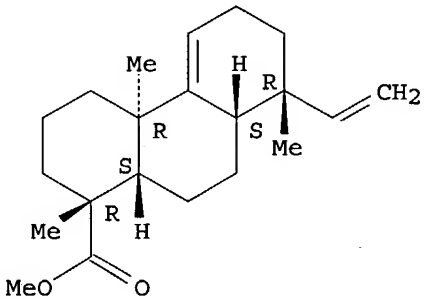
Absolute stereochemistry. Rotation (-).



RN 308795-78-0 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

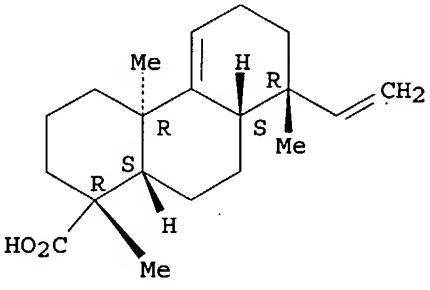
Absolute stereochemistry.



RN 308795-79-1 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

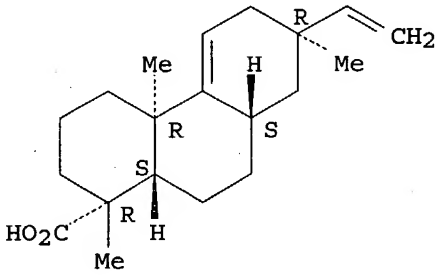


IT **60855-32-5P 119290-87-8P**, (-)-Acanthoic acid

467221-99-4P 467222-00-0P 467222-01-1P
467222-02-2P 467222-03-3P 467222-04-4P
467222-05-5P 467222-06-6P 467222-07-7P
467222-08-8P 467222-09-9P 467222-11-3P
467222-12-4P 467222-13-5P 467222-14-6P
467222-15-7P 467222-16-8P 467222-17-9P
467222-18-0P 467222-19-1P 467222-20-4P
467222-21-5P 467222-22-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

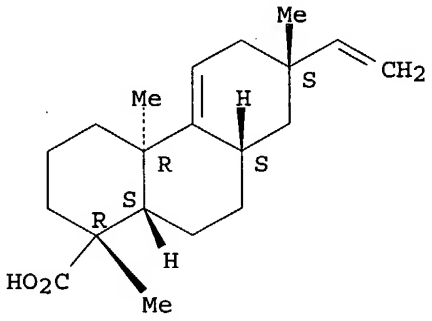
RN 60855-32-5 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



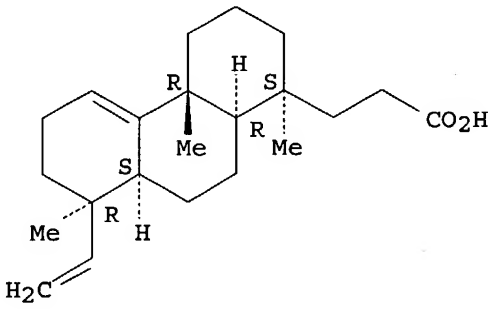
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



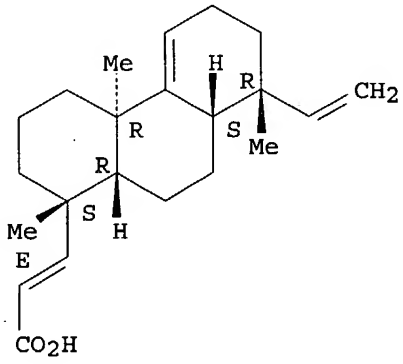
RN 467221-99-4 HCAPLUS
CN 1-Phenanthrenepropanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



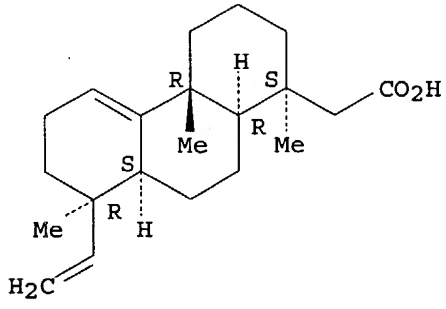
RN 467222-00-0 HCAPLUS
CN 2-Propenoic acid, 3-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



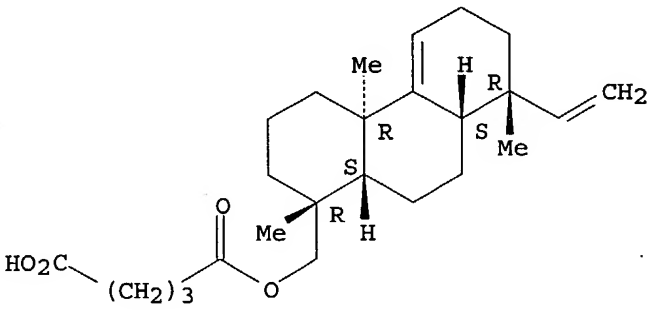
RN 467222-01-1 HCAPLUS
CN 1-Phenanthreneacetic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



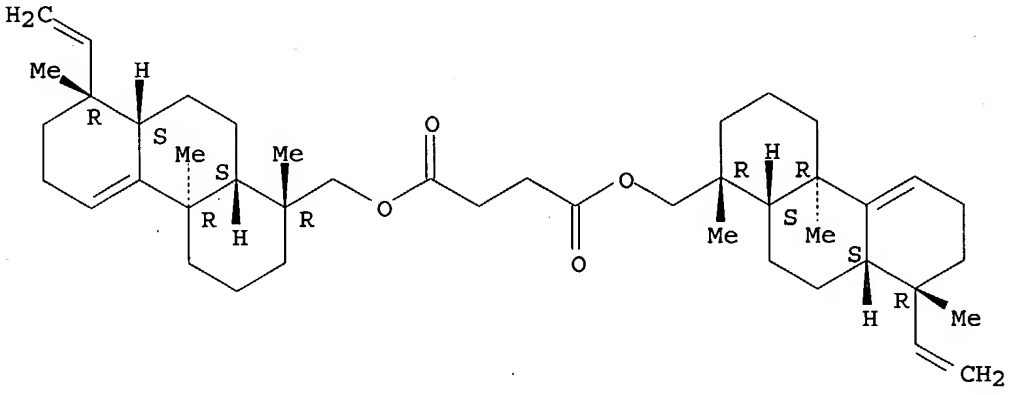
RN 467222-02-2 HCAPLUS
CN Pentanedioic acid, mono[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



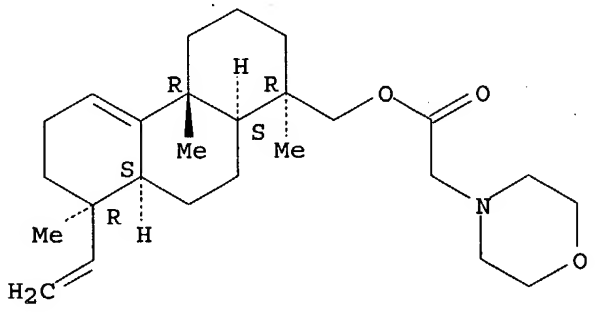
RN 467222-03-3 HCAPLUS
CN Butanedioic acid, bis[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



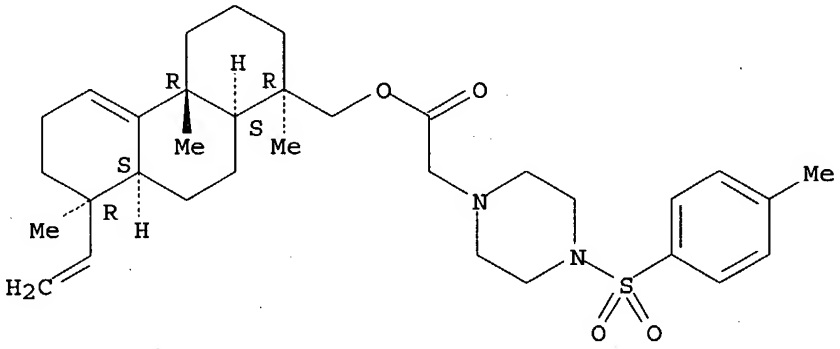
RN 467222-04-4 HCAPLUS
CN 4-Morpholineacetic acid, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



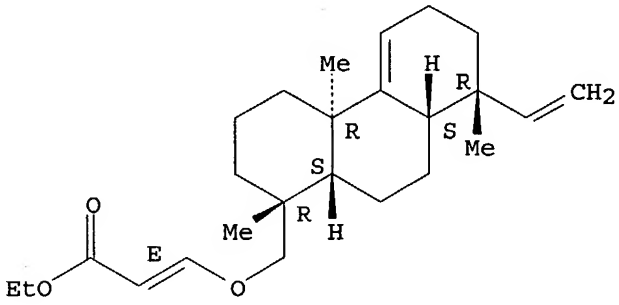
RN 467222-05-5 HCAPLUS
CN 1-Piperazineacetic acid, 4-[(4-methylphenyl)sulfonyl]-, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



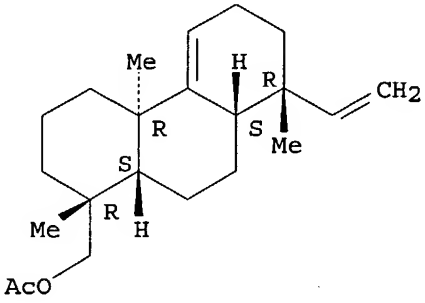
RN 467222-06-6 HCAPLUS
CN 2-Propenoic acid, 3-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methoxy]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



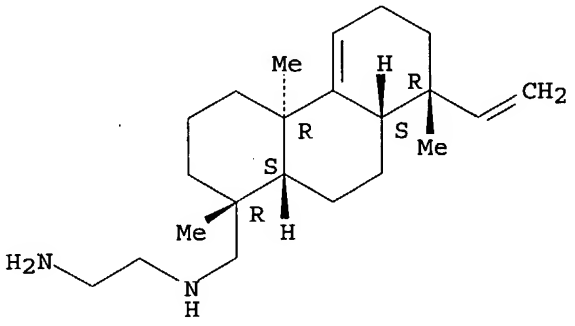
RN 467222-07-7 HCAPLUS
CN 1-Phenanthrenemethanol, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, acetate, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



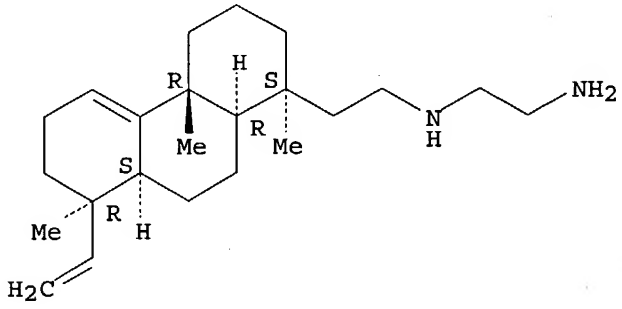
RN 467222-08-8 HCAPLUS
CN 1,2-Ethanediamine, N-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



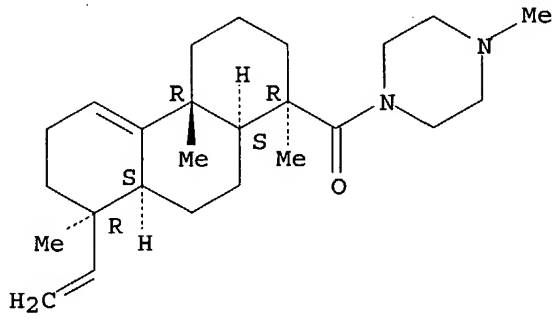
RN 467222-09-9 HCAPLUS
CN 1,2-Ethanediamine, N-[2-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



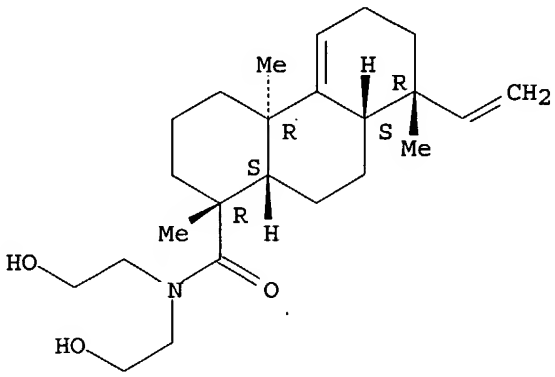
RN 467222-11-3 HCAPLUS
CN Piperazine, 1-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



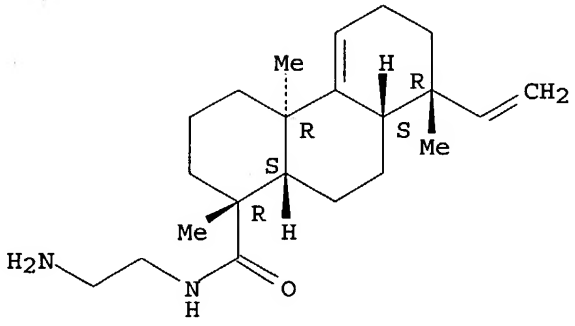
RN 467222-12-4 HCAPLUS
CN 1-Phenanthrenecarboxamide, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-N,N-bis(2-hydroxyethyl)-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



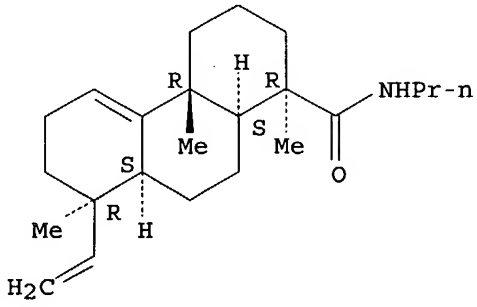
RN 467222-13-5 HCAPLUS
CN 1-Phenanthrenecarboxamide, N-(2-aminoethyl)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



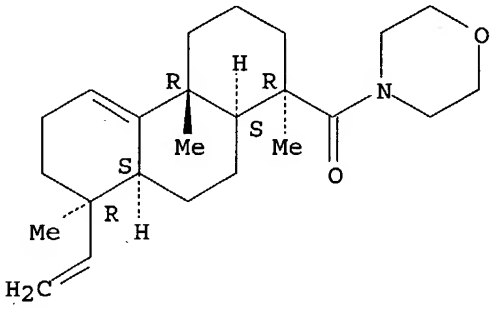
RN 467222-14-6 HCAPLUS
CN 1-Phenanthrenecarboxamide, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-N-propyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



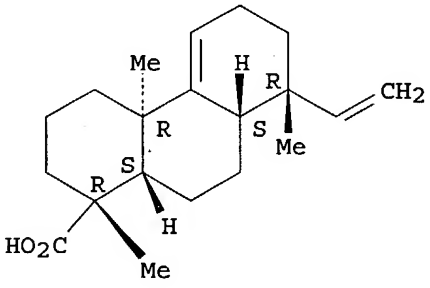
RN 467222-15-7 HCAPLUS
CN Morpholine, 4-[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 467222-16-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, potassium salt, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

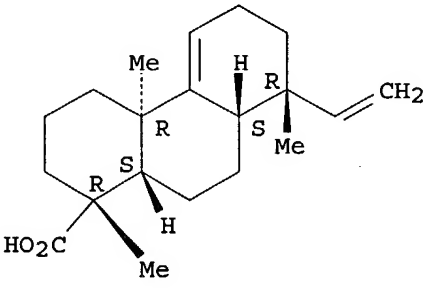
Absolute stereochemistry.



● K

RN 467222-17-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, sodium salt, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

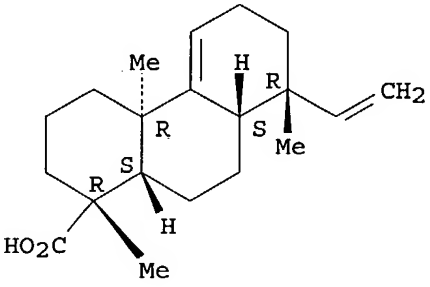
RN 467222-18-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)-, compd. with

2,2',2''-nitrilotris[ethanol] (1:1) (9CI) (CA INDEX NAME)

CM 1

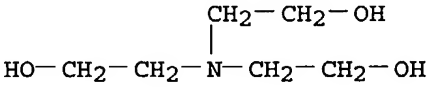
CRN 308795-79-1
CMF C20 H30 O2

Absolute stereochemistry.



CM 2

CRN 102-71-6
CMF C6 H15 N O3

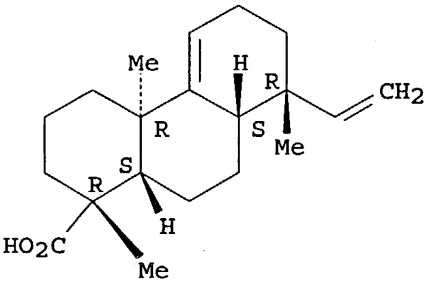


RN 467222-19-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)-, compd. with 2,2'-iminobis[ethanol] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 308795-79-1
CMF C20 H30 O2

Absolute stereochemistry.



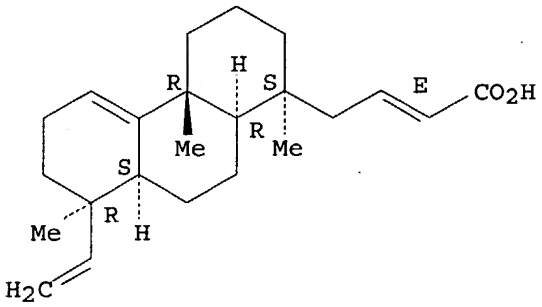
CM 2

CRN 111-42-2
CMF C4 H11 N O2

HO—CH_2—CH_2—NH—CH_2—CH_2—OH

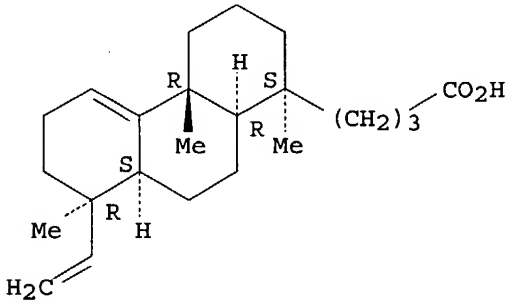
RN 467222-20-4 HCAPLUS
CN 2-Butenoic acid, 4-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



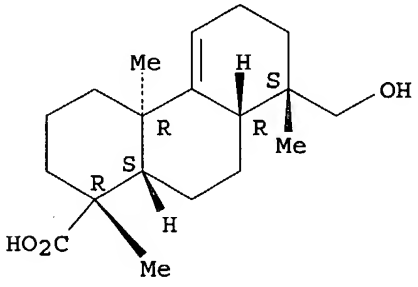
RN 467222-21-5 HCAPLUS
CN 1-Phenanthrenebutanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 467222-22-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

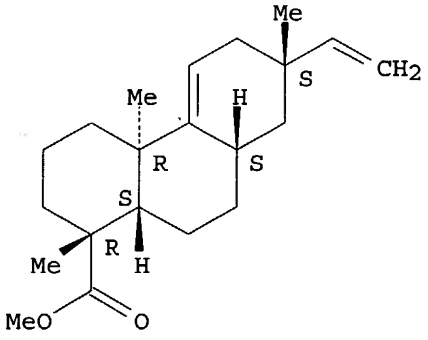
Absolute stereochemistry.



IT **103462-23-3P 308795-77-9P 308795-83-7P**
467222-23-7P 467222-24-8P 467222-26-0P
467222-28-2P 467222-29-3P 467222-30-6P
467222-31-7P 467222-32-8P 467222-33-9P
467222-34-0P 467222-35-1P 467222-36-2P
467222-39-5P 467222-40-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)

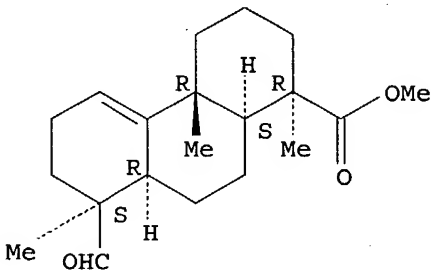
RN 103462-23-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



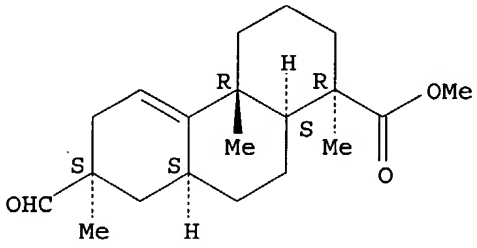
RN 308795-77-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



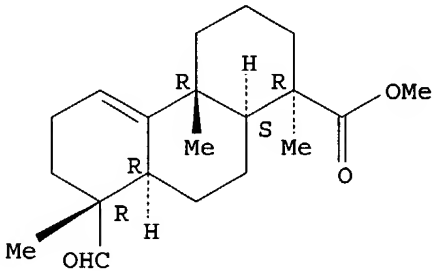
RN 308795-83-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



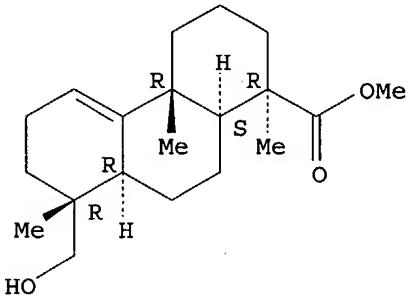
RN 467222-23-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



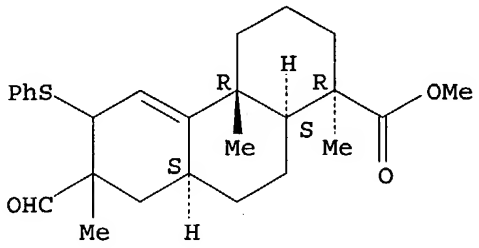
RN 467222-24-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



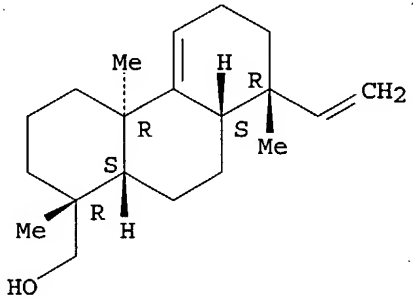
RN 467222-26-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-6-(phenylthio)-, methyl ester, (1R,4aR,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



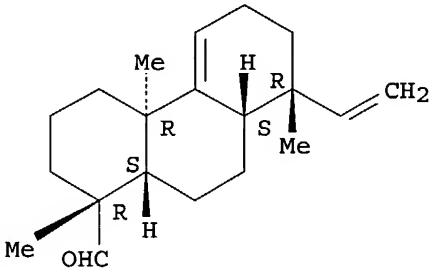
RN 467222-28-2 HCAPLUS
CN 1-Phenanthrenemethanol, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



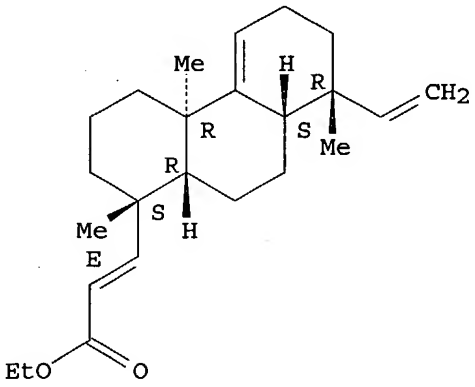
RN 467222-29-3 HCAPLUS
CN 1-Phenanthrenecarboxaldehyde, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



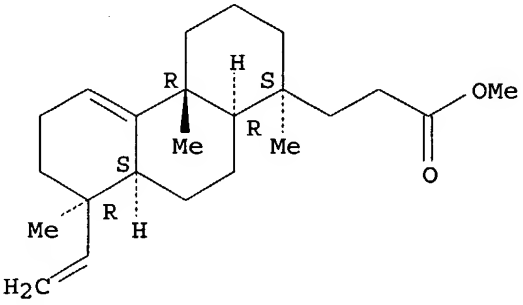
RN 467222-30-6 HCAPLUS
CN 2-Propenoic acid, 3-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



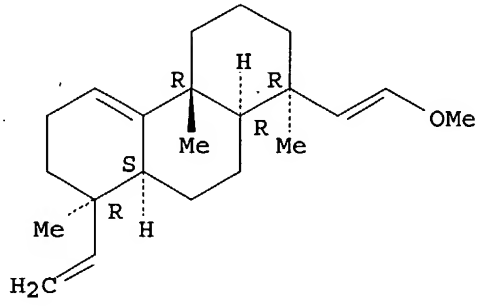
RN 467222-31-7 HCAPLUS
CN 1-Phenanthrenepropanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



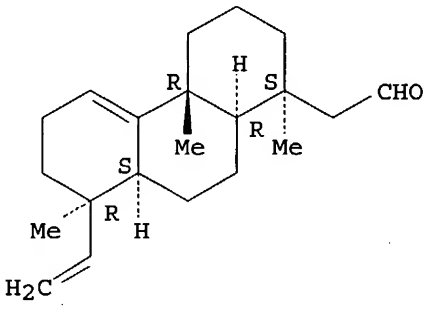
RN 467222-32-8 HCAPLUS
CN Phenanthrene, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1-(2-methoxyethenyl)-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



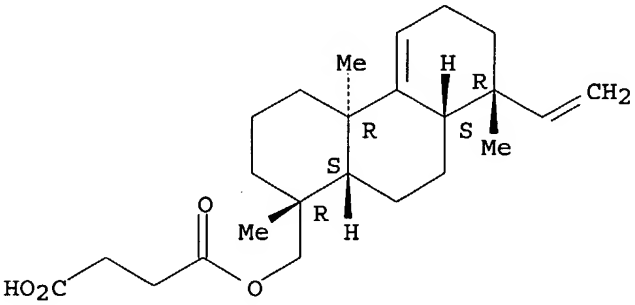
RN 467222-33-9 HCAPLUS
CN 1-Phenanthreneacetaldehyde, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



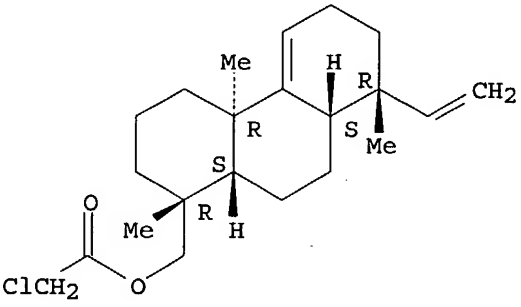
RN 467222-34-0 HCAPLUS
CN Butanedioic acid, mono[[(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



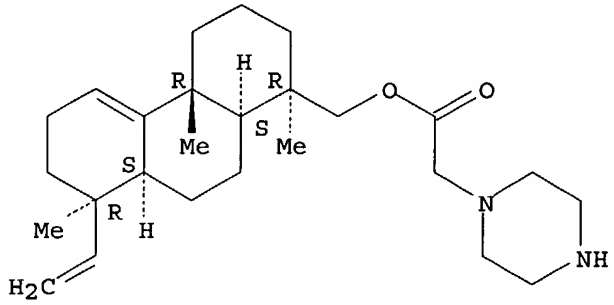
RN 467222-35-1 HCAPLUS
CN Acetic acid, chloro-, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



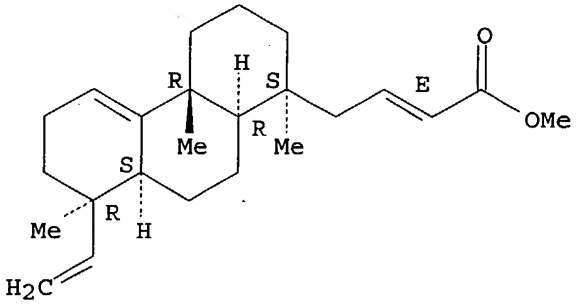
RN 467222-36-2 HCAPLUS
CN 1-Piperazineacetic acid, [(1R,4aR,8R,8aS,10aS)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



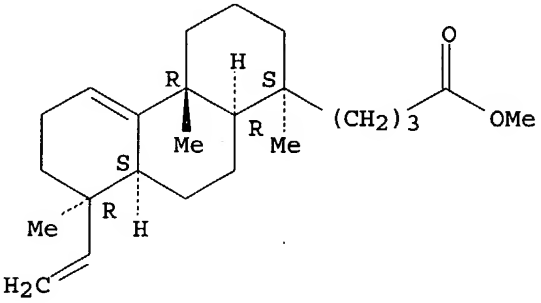
RN 467222-39-5 HCAPLUS
CN 2-Butenoic acid, 4-[(1S,4aR,8R,8aS,10aR)-8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-1-phenanthrenyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



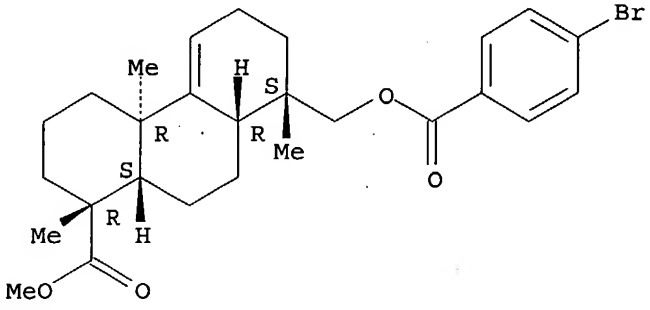
RN 467222-40-8 HCAPLUS
CN 1-Phenanthrenebutanoic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1S,4aR,8R,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



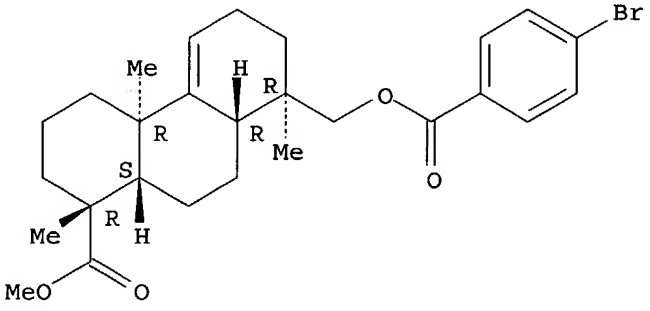
IT **287401-15-4P 467222-27-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of interleukin-1 and tumor necrosis factor-α modulators)
RN 287401-15-4 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 467222-27-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:847200 HCAPLUS
DN 136:118594
ED Entered STN: 22 Nov 2001
TI Enantioselective Synthesis of the Antiinflammatory Agent (-)-Acanthoic Acid
AU Ling, Taotao; Chowdhury, Chinmay; Kramer, Bryan A.; Vong, Binh G.; **Palladino, Michael A.; Theodorakis, Emmanuel A.**
CS Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA, 92093-0358, USA
SO Journal of Organic Chemistry (2001), 66(26), 8843-8853
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 30-20 (Terpenes and Terpenoids)
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB An enantioselective synthesis of the potent antiinflammatory agent (-)-acanthoic acid (I) is described. The successful strategy departs from (-)-Wieland-Miescher ketone (II), which is readily available in both enantiomeric forms and constitutes the starting point toward a fully

functionalized AB ring system of I. Conditions were developed for a regioselective double alkylation at the C4 center of the A ring, which produced compound III as a single stereoisomer. Construction of the C ring of I was accomplished via a Diels-Alder reaction between sulfur-containing diene IV and methacrolein, which after desulfurization and further functionalization yielded synthetic acanthoic acid. The described synthesis confirms the proposed stereochem. of the natural product and represents a fully stereocontrolled entry into an under explored class of biol. active diterpenes.

ST diterpene acanthoic acid asym synthesis regioselective double alkylation; crystal structure multicyclic intermediate acanthoic acid asym synthesis; Diels Alder reaction acanthoic acid asym synthesis

IT Diels-Alder reaction
(between a sulfur containing diene and methacrolein in the asym. synthesis of enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

IT Asymmetric synthesis and induction
(enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

IT Diterpenes
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective synthesis of the diterpenoid antiinflammatory agent (-)-acanthoic acid)

IT Crystal structure
(of multicyclic synthetic intermediates of the antiinflammatory agent (-)-acanthoic acid)

IT Alkylation
(regioselective double; enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid via)

IT 287401-07-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure; enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

IT **287401-15-4P 287401-16-5P** 391277-77-3P 391277-79-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

IT 78-85-3 107-02-8, 2-Propenal, reactions 108-98-5, Thiophenol, reactions 141-78-6, Acetic acid ethyl ester, reactions 1193-55-1 100348-93-4 132836-66-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

IT 3733-18-4P 22418-80-0P 38996-01-9P 82273-33-4P **103462-23-3P** 117556-90-8P **187722-32-3P** 187750-47-6P 287401-06-3P 287401-08-5P 287401-09-6P 287401-10-9P 287401-11-0P **287401-12-1P 287401-13-2P 287401-14-3P** **287401-17-6P 287478-47-1P** 391277-72-8P 391277-73-9P 391277-74-0P 391277-76-2P 391277-80-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

IT **119290-87-8P 308795-77-9P 308795-84-8P** 391277-75-1P 391277-78-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

RE.CNT 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Aggarwal, B; Human Cytokines:Their Role in Disease and Therapy 1995
(2) Antonaroli, S; Gazz Chim Ital 1992, V122, P55 HCAPLUS

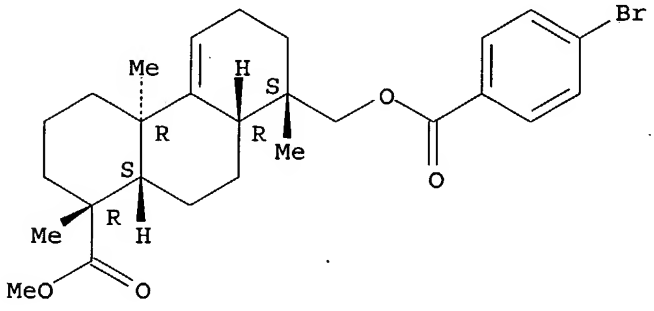
(3) Apsimon, J; The Total Synthesis of Natural Products 1990, V8
(4) Barnier, J; Tetrahedron:Asymmetry 1999, V10, P1107 HCAPLUS
(5) Barton, D; J Chem Soc, Perkin Trans 1 1975, P1574 HCAPLUS
(6) Bennet, C; Tetrahedron 1967, V23, P927
(7) Beutler, B; Tumor Necrosis Factors The Molecules and Their Emerging Role in Medicine 1992
(8) Brader, G; Phytochemistry 1997, V45, P1207 HCAPLUS
(9) Buchschacher, P; Org Synth Coll 1990, VVII, P368
(10) Camussi, G; Drugs 1998, V55, P613 HCAPLUS
(11) Caselli, A; Aust J Chem 1982, V35, P799 HCAPLUS
(12) Coates, R; J Org Chem 1970, V35, P2597 HCAPLUS
(13) Coates, R; J Org Chem 1970, V35, P2601 HCAPLUS
(14) Cohen, T; J Org Chem 1982, V47, P4008
(15) Coisne, J; Bull Soc Chim Belg 1980, V89, P551 HCAPLUS
(16) Crabtree, S; Org Synth 1992, V70, P256 HCAPLUS
(17) Cragg, G; J Nat Prod 1997, V60, P52 HCAPLUS
(18) Cragg, G; Med Res Rev 1998, V18, P315 HCAPLUS
(19) Das, J; Can J Chem 1979, V57, P3308 HCAPLUS
(20) Das, J; Can J Chem 1984, V62, P1103 HCAPLUS
(21) Das, J; Can J Chem 1984, V62, P1103 HCAPLUS
(22) Dess, D; J Am Chem Soc 1991, V113, P7277 HCAPLUS
(23) Dev, S; CRC Handbook of Terpenoids 1986
(24) Dumortier, L; Tetrahedron Lett 1989, V30, P3201 HCAPLUS
(25) Evans, D; Aldrichimica Acta 1982, V15, P23 HCAPLUS
(26) Evans, D; Angew Chem, Int Ed Engl 1997, V36, P2119 HCAPLUS
(27) Farnsworth, N; Bull WHO 1985, V63, P965 MEDLINE
(28) Galvani, D; Cytokine Therapy 1992
(29) Ge, M; Org Lett 2000, V2, P1927 HCAPLUS
(30) Gemal, A; J Am Chem Soc 1981, V103, P5454 HCAPLUS
(31) Glasby, J; Encyclopaedia of the Terpenoids 1982, V1-2
(32) Grabley, S; Drug Discovery from Nature 2000
(33) Greengrass, C; J Chem Soc, Chem Commun 1985, P889 HCAPLUS
(34) Gullo, V; The Discovery of Natural Products with Therapeutic Potential 1994
(35) Hopkins, P; J Org Chem 1978, V43, P1208 HCAPLUS
(36) Ireland, R; J Org Chem 1993, V58, P2899 HCAPLUS
(37) Ireland, R; Tetrahedron Lett 1960, V25, P37
(38) Joel, S; Chem Ind 1994, P172 HCAPLUS
(39) Jung, M; Tetrahedron 1976, V32, P3 HCAPLUS
(40) Kakushima, M; Can J Chem 1979, V57, P3354 HCAPLUS
(41) Kakushima, M; Can J Chem 1979, V57, P3356 HCAPLUS
(42) Kang, H; Cellular Immunol 1996, V170, P212 HCAPLUS
(43) Kang, H; Mediators Inflamm 1998, V7, P257 HCAPLUS
(44) Kaufman, P; Natural Products from Plants 1999
(45) Kim, Y; J Nat Prod 1988, V51, P1080 HCAPLUS
(46) Kinghorn, A; Human Medicinal Agents from Plants; ACS Symposium Series 534 1993
(47) Kobuke, Y; J Am Chem Soc 1970, V92, P6548
(48) Kolaczkowski, L; J Org Chem 1985, V50, P4766 HCAPLUS
(49) Kurzrock, R; Cytokines:Interleukins and Their Receptors 1995
(50) Lee, J; J Org Chem 1992, V57, P5301 HCAPLUS
(51) Lee, K; J Biomed Sci 1999, V6, P236 HCAPLUS
(52) Lee, K; Med Res Rev 1999, V19, P569 HCAPLUS
(53) Ling, T; Angew Chem, Int Ed 1999, V38, P3089 HCAPLUS
(54) Ling, T; Org Lett 2000, V2, P2073 HCAPLUS
(55) Mehta, G; J Am Chem Soc 1986, V108, P3443 HCAPLUS
(56) Minuti, L; Synth Comm 1992, V22, P1535 HCAPLUS
(57) Nakanishi, K; Natural Products Chemistry 1974, V1
(58) Nazarov, I; Zh Obshch Khim 1953, V23, P1703 HCAPLUS
(59) Newman, D; Nat Prod Rep 2000, V17, P215 HCAPLUS
(60) Newton, R; J Med Chem 1999, V42, P2295 HCAPLUS
(61) Nisbet, L; Curr Opin Biotechn 1997, V8, P708 HCAPLUS
(62) Oppolzer, W; Comprehensive Org Synthesis 1991, P315

(63) Overman, L; J Am Chem Soc 1983, V105, P6335 HCAPLUS
(64) Padwa, A; J Org Chem 1990, V55, P4144 HCAPLUS
(65) Pandley, R; Med Res Rev 1998, V18, P333
(66) Perry, L; Medicinal Plants of East and Southeast Asia 1980
(67) Petrzilka, M; Synthesis 1981, P753 HCAPLUS
(68) Ruzicka, L; J Am Chem Soc 1948, V70, P2081
(69) Schkeryantz, J; Synlett 1998, P723 HCAPLUS
(70) Schuster, T; Org Lett 2000, V2, P179 HCAPLUS
(71) Shu, Y; J Nat Prod 1998, V61, P1053 HCAPLUS
(72) Stork, G; J Am Chem Soc 1965, V87, P275 HCAPLUS
(73) Stork, G; Tetrahedron Lett 1972, P2755 HCAPLUS
(74) Suffness, M; Ann Rep Med Chem 1993, V28, P305 HCAPLUS
(75) Suh, Y; Arch Pharm Res 1995, V18, P217 HCAPLUS
(76) Suh, Y; Synth Commun 1997, V27, P587 HCAPLUS
(77) Szekanecz, Z; Clinical Pharmacol 1998, V12, P377 MEDLINE
(78) Thorpe, R; Cytokines 1998
(79) Trost, B; J Am Chem Soc 1977, V99, P8116 HCAPLUS
(80) Trost, B; J Am Chem Soc 1980, V102, P7910 HCAPLUS
(81) Wall, M; Med Res Rev 1998, V18, P299 HCAPLUS
(82) Watson, A; J Org Chem 1995, V60, P5102 HCAPLUS
(83) Welch, S; J Am Chem Soc 1977, V99, P549 HCAPLUS
(84) Welch, S; J Org Chem 1977, V42, P2879 HCAPLUS
(85) Welch, S; Synth Comm 1973, V3, P29 HCAPLUS
(86) Wenkert, E; J Am Chem Soc 1959, V81, P688 HCAPLUS
(87) Wenkert, E; J Am Chem Soc 1964, V86, P2038 HCAPLUS
(88) Wenkert, E; J Am Chem Soc 1972, V94, P4367 HCAPLUS
(89) Woodward, R; Tetrahedron 1959, V5, P70 HCAPLUS
(90) Xiang, A; J Org Chem 1998, V63, P6774 HCAPLUS
(91) Yoon, T; Angew Chem, Int Ed Engl 1994, V33, P853
(92) Zibuck, R; J Org Chem 1989, V54, P4717 HCAPLUS
(93) Zibuck, R; Org Synth 1993, V71, P236 HCAPLUS

IT **287401-15-4P 287401-16-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

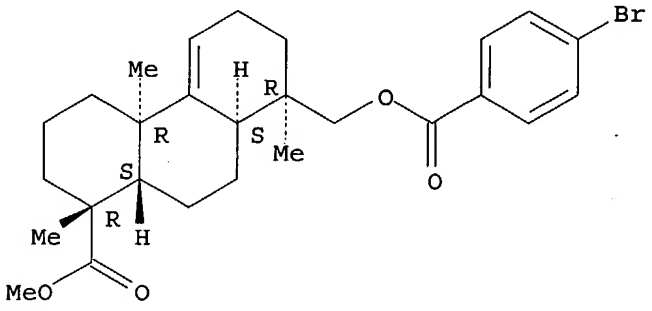
RN 287401-15-4 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 287401-16-5 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

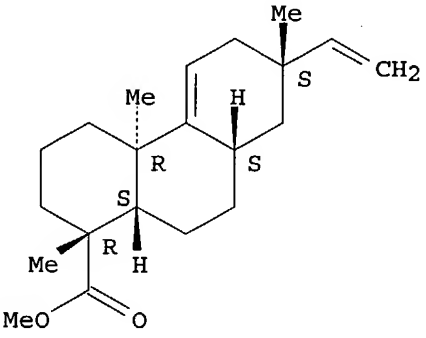
Absolute stereochemistry. Rotation (+).



IT **103462-23-3P 187722-32-3P 287401-12-1P 287401-13-2P 287401-14-3P 287401-17-6P 287478-47-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)

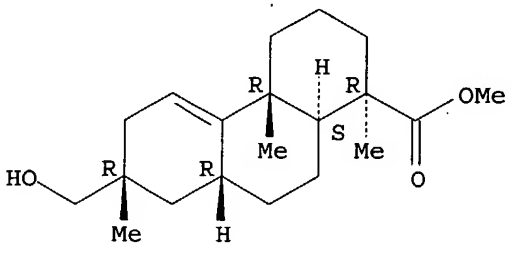
RN 103462-23-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 187722-32-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(hydroxymethyl)-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7R,8aR,10aS)- (9CI) (CA INDEX NAME)

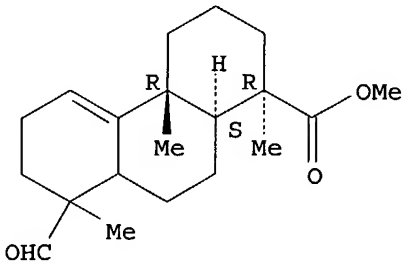
Absolute stereochemistry. Rotation (-).



RN 287401-12-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,10aS)- (9CI) (CA

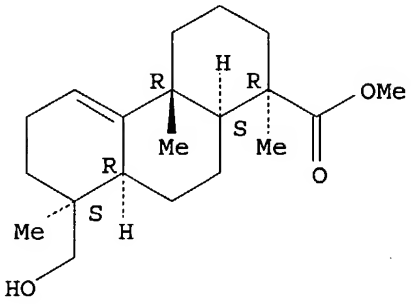
INDEX NAME)

Absolute stereochemistry.



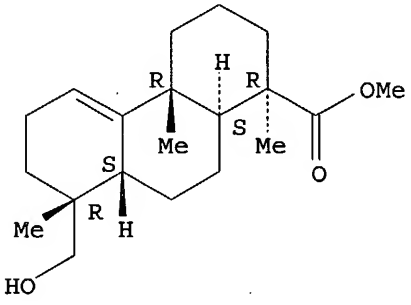
RN 287401-13-2 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



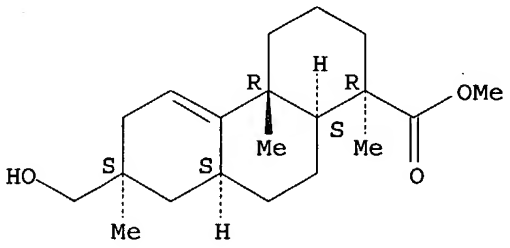
RN 287401-14-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



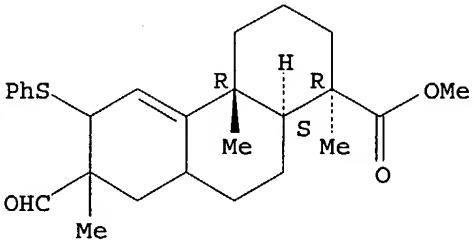
RN 287401-17-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(hydroxymethyl)-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



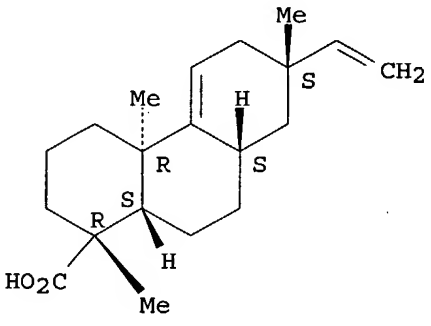
RN 287478-47-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-6-(phenylthio)-, methyl ester, (1R,4aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



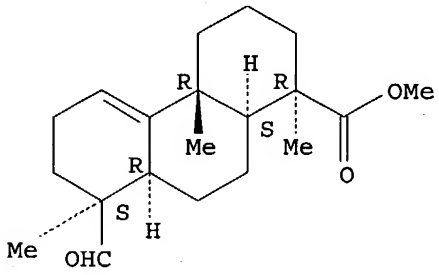
IT **119290-87-8P 308795-77-9P 308795-84-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective synthesis of the antiinflammatory agent (-)-acanthoic acid)
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



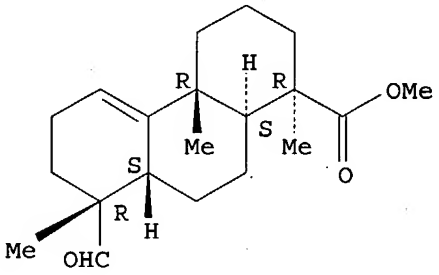
RN 308795-77-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 308795-84-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L50 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:703740 HCAPLUS
DN 135:251986
ED Entered STN: 26 Sep 2001
TI Methods for treating fibroproliferative diseases with antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides
IN Peterson, Theresa C.
PA Dalhousie University, Can.
SO U.S., 13 pp., Cont.-in-part of U.S. 6,025,151.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C12Q001-02
ICS C12Q001-00; C12Q001-50
NCL 435029000
CC 1-12 (**Pharmacology**)
Section cross-reference(s): 9, **63**
FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6294350	B1	20010925	US 1999-433621	19991102 <--
US 5985592	A	19991116	US 1997-870096	19970605 <--
US 6025151	A	20000215	US 1998-92317	19980605 <--
WO 2001032156	A2	20010510	WO 2000-IB1731	20001102
WO 2001032156	A3	20020926		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 1997-870096 A2 19970605 <--
US 1998-92317 A2 19980605 <--
US 1999-433621 A1 19991102

AB In accordance with the present invention, fibroproliferative disease or condition characterized by such symptoms as increased levels of c-Jun homodimers, increased heterodimerization of c-Jun with another signaling peptide, increased levels of phosphorylated c-Jun, or increased presence of Jun kinase are treated by administering to the subject an amount of a compound effective to ameliorate one or more of the symptoms of the disease or condition, for example, an antiproliferative or antifibrotic agent. Preferred compds. for administration according to the invention are antisense c-Jun oligonucleotides and compds. that block c-Jun phosphorylation, such as pentoxifylline, or a functional derivative or metabolite thereof. Also provided by the present invention are in vitro tests for identifying whether a test compound is useful for treatment of a subject afflicted with such a disease and kits useful for conducting such assays.

ST fibroproliferative disease treatment antiproliferative antifibrotic agent; antiproliferative antisense oligonucleotide fibroproliferative disease cJun

IT Peptides, biological studies
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(ATF2; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Angiotensin receptors
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(AT1, inhibitors; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Hepatitis
(C; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Transcription factors
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CREB (cAMP-responsive element-binding); antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Eye, disease
Graves' disease
(Graves' ophthalmopathy; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Sarcoma
(Kaposi's; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Neoplasm
(Li-Fraumeni syndrome; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Transcription factors
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL

(Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(NF-κB (nuclear factor κB); antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Peptides, biological studies
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Nrf1; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Eye
(Tenon's capsule, fibroproliferation; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Leukemia
(acute myelogenous; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Abdomen
(adhesions; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Fibrosis
(antifibrotics; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Alzheimer's disease
Animal tissue culture
Anti-Alzheimer's agents
Antitumor agents
Drug screening
Epithelium
Fibroblast
Hematopoietic precursor cell
Keloid
Kidney, disease
Leprosy
Mesenchyme
Multiple sclerosis
Myelodysplastic syndromes
Myeloproliferative disorders
Neoplasm
Neuroglia
Phosphorylation, biological
Picrorhiza kurroa
Signal transduction, biological
Silicosis
Silybum marianum
Test kits
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Platelet-derived growth factors
Tumor necrosis factors
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Antisense oligonucleotides
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Decorins
Phosphatidylcholines, biological studies
Tocopherols
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Bronchi
(bronchiolitis, obliterative; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Signal peptides
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence); PROC (Process)
(c-Jun heterodimerization with; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Transcription factors
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BPN (Biosynthetic preparation); BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(c-jun; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Malaria
(cerebral; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Intestine, disease
(colitis, collagenous; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Cardiovascular system
(disease; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Drugs
Ergot (Claviceps)
(drug-induced ergotism; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Reproductive tract
(female, cancer; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Intestine
Lung
Skin
(fibroblasts of; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Radiation
(fibrosis from; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Heart, disease
Kidney, disease
Liver, disease
Lung, disease
Peritoneum
(fibrosis; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Gene, animal
RL: BPN (Biosynthetic preparation); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation); PROC (Process)
(for c-Jun; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Neuroglia
(glioblastoma, sporadic; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Neuroglia
(glioblastoma; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Kidney, disease
(glomerulonephritis; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Neutrophil
(infiltration; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Intestine, disease
(inflammatory; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Cytokines
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(inflammatory; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Drug delivery systems
(inhalants; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Drug delivery systems
(injections, i.m.; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Drug delivery systems
(injections, i.v.; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Lung, disease
(interstitial; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Brain, disease
(malaria; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Antitumor agents
(mammary gland; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Kidney
(mesangium; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Leukemia
(myelogenous; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)
IT Liver

(myofibroblasts of; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Mammary gland
(neoplasm, inhibitors; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Mammary gland
(neoplasm; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Nerve, neoplasm
(neuroblastoma; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Drug delivery systems
(oral; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Proteins, specific or class
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(p65, NF-κB p65; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Phosphatidylcholines, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polyenyl-; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Proliferation inhibition
(proliferation inhibitors; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Disease, animal
(proliferative; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Drug delivery systems
(rectal; antiproliferative or antifibrotic agents, especially antisense c-Jun
oligonucleotides, for treating fibroproliferative diseases)

IT Connective tissue
(scleroderma; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Shock (circulatory collapse)
(septic; antiproliferative or antifibrotic agents, especially antisense c-Jun
oligonucleotides, for treating fibroproliferative diseases)

IT Blood vessel
(smooth muscle; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Muscle
(smooth; antiproliferative or antifibrotic agents, especially antisense c-Jun
oligonucleotides, for treating fibroproliferative diseases)

IT Carcinoma
(squamous cell, differentiation disorder; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Cell differentiation
(squamous cell, disorder; antiproliferative or antifibrotic agents,

especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Drug delivery systems
(sustained-release; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Lupus erythematosus
(systemic, nephritis associated with; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Drug delivery systems
(topical; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Drug delivery systems
(transdermal; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Interferons
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(α; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT Transforming growth factors
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(β-, RII/FC; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT 155215-87-5, Jun kinase
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT 217308-10-6, DNA, d(G-C-A-G-T-C-A-T-A-G-A-A-C-A-G-T-C-C-G-T-C-A-C-T-T-C-A-C-G-T)
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT 50-23-7, Hydrocortisone 54-85-3, Isoniazid 54-85-3D, Isoniazid, conjugated 59-67-6, Niacin, biological studies 64-86-8, Colchicine 107-35-7, Taurine 518-34-3, Tetrandrine 1028-33-7, Pentifylline 1405-86-3, Glycyrrhizin 6493-05-6, Pentoxifylline 6493-05-6D, Pentoxifylline, derivs. and metabolites 6493-06-7, 1H-Purine-2,6-dione, 3,7-dihydro-1-(5-hydroxyhexyl)-3,7-dimethyl- 10102-43-9, Nitric oxide, biological studies 53179-13-8, Pirfenidone 55242-55-2, Propentofylline 55837-20-2, Halofuginone 62571-86-2, Captopril 75847-73-3, Enalapril 80288-49-9, Furafylline 83150-76-9, Octreotide 85721-33-1, Ciprofloxacin 91161-71-6, Terbinafine 114798-26-4, Losartan **119290-87-8**, Acanthoic acid 120210-48-2, Tenidap
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT 50-88-4, Tritiated thymidine, biological studies 1148-63-6, Thymidine-α-t 42459-79-0, Uridine, 5-bromo-, labeled with tritium
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL

(Biological study); PROC (Process); USES (Uses)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT 330196-64-0, Cytochrome p 450 1A2
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(inhibitors; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

IT 9015-82-1, Angiotensin converting enzyme
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

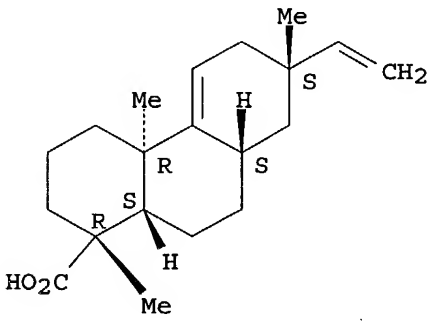
(1) Anon; DE 3604149 A1 1987 HCAPLUS
(2) Anon; WO 8700523 A2 1987 HCAPLUS
(3) Anon; WO 9219772 A1 1992 HCAPLUS
(4) Anon; EP 0544391 A1 1993 HCAPLUS
(5) Anon; WO 9502051 A2 1995 HCAPLUS
(6) Anon; WO 9526727 A1 1995 HCAPLUS
(7) Bamberger; Proc Natl Acad Sci USA 1996, V93, P6169 HCAPLUS
(8) Bessler; J Leukocyte Biol 1986, V40, P747 HCAPLUS
(9) Bianco; US 5585380 1996 HCAPLUS
(10) Bonsen; US 4265874 1981 HCAPLUS
(11) Peterson; US 5985592 1999 HCAPLUS
(12) Peterson; US 6025151 2000 HCAPLUS
(13) Theeuwes; US 4160452 1979 HCAPLUS
(14) Theeuwes; US 4256108 1981

IT **119290-87-8**, Acanthoic acid
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(antiproliferative or antifibrotic agents, especially antisense c-Jun oligonucleotides, for treating fibroproliferative diseases)

RN 119290-87-8 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:338333 HCAPLUS

DN 134:357558

ED Entered STN: 11 May 2001

TI Methods for treating fibroproliferative diseases

IN Peterson, Theresa C.

PA Dalhousie University, Can.

SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM A61K031-00
ICS A61K031-522; A61K045-00; A61K045-06; A61K048-00; C12Q001-48; G01N033-58; A61P019-04; A61P035-00; A61P037-00; A61P025-28; A61P043-00; A61P033-06; A61P031-12; A61P039-00; A61P035-02; A61P001-00; A61P011-00; A61P013-12; A61P009-00
CC 63-6 (**Pharmaceuticals**)
Section cross-reference(s): **1**, 2, 8, 15
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001032156	A2	20010510	WO 2000-IB1731	20001102
	WO 2001032156	A3	20020926		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6294350	B1	20010925	US 1999-433621	19991102 <--
PRAI	US 1999-433621	A1	19991102		
	US 1997-870096	A2	19970605 <--		
	US 1998-92317	A2	19980605 <--		

AB In accordance with the present invention, fibroproliferative disease or condition characterized by such symptoms as increased levels of c-Jun homodimers, increased heterodimerization ofc-Jun with another signaling peptide, increased levels of phosphorylated c-Jun, or increased presence of Jun kinase are treated by administering to the subject an amount of a compound effective to ameliorate one or more of the symptoms of the disease or condition, for example, an antiproliferative or antifibrotic agent. Preferred compds. for administration according to the invention are antisense c-Jun oligonucleotides and compds. that block c-Jun phosphorylation, such as pentoxifylline, or a functional derivative or metabolite thereof. Also provided by the present invention are in vitro tests for identifying whether a test compound is useful for treatment of a subject afflicted with such a disease and kits useful for conducting such assays.

ST antiproliferative antisense oligonucleotide fibroproliferative disease cJun

IT Peptides, biological studies
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(ATF2; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Angiotensin receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(AT1, inhibitors; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Hepatitis
(C; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Transcription factors
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CREB (cAMP-responsive element-binding); antisense oligonucleotide

prepns. for treating fibroproliferative diseases)
IT Eye, disease
Graves' disease
(Graves' ophthalmopathy; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Sarcoma
(Kaposi's; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Neoplasm
(Li-Fraumeni syndrome; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Transcription factors
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(NF-κB (nuclear factor κB); antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Peptides, biological studies
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Nrf1; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Eye
(Tenon's capsule, fibroproliferation; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Leukemia
(acute myelogenous; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Abdomen
(adhesions; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Fibrosis
(antifbrotics; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Alzheimer's disease
Animal tissue culture
Anti-Alzheimer's agents
Antitumor agents
Epithelium
Fibroblast
Hematopoietic precursor cell
Keloid
Kidney, disease
Leprosy
Mesenchyme
Multiple sclerosis
Myelodysplastic syndromes
Myeloproliferative disorders
Neoplasm
Neuroglia
Phosphorylation, biological
Picrorhiza kurroa
Signal transduction, biological
Silicosis
Silybum marianum
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Platelet-derived growth factors
Tumor necrosis factors
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)

(antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Antisense oligonucleotides
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Decorins
Phosphatidylcholines, biological studies
Tocopherols
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Bronchi
(bronchiolitis, obliterative; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Transcription factors
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(c-jun; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Malaria
(cerebral; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Intestine, disease
(colitis, collagenous; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Cardiovascular system
(disease; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Reproductive tract
(female, cancer; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Intestine
Lung
Skin
(fibroblasts of; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Radiation
(fibrosis from; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Heart, disease
Kidney, disease
Lung, disease
Peritoneum
(fibrosis; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Neuroglia
(glioblastoma, sporadic; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Neuroglia
(glioblastoma; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Kidney, disease
(glomerulonephritis; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Neutrophil
(infiltration; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Intestine, disease
(inflammatory; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Cytokines
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(inflammatory; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(inhalants; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(injections, i.m.; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(injections, i.v.; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Lung, disease
(interstitial; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Brain, disease
(malaria; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Antitumor agents
(mammary gland; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Kidney
(mesangium; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Leukemia
(myelogenous; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Liver
(myofibroblasts of; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Mammary gland
(neoplasm, inhibitors; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Mammary gland
(neoplasm; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Nerve, neoplasm
(neuroblastoma; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(oral; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Proteins, specific or class
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(p65; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Phosphatidylcholines, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polyenyl-; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Proliferation inhibition
(proliferation inhibitors; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT Disease, animal
(proliferative; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(rectal; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Connective tissue
(scleroderma; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Shock (circulatory collapse)
(septic; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Blood vessel
(smooth muscle; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Muscle
(smooth; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Carcinoma
(squamous cell, differentiation disorder; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Cell differentiation
(squamous cell, disorder; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(sustained-release; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Lupus erythematosus
(systemic, nephritis; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(topical; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Drug delivery systems
(transdermal; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Interferons
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(α; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT Transforming growth factors
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(β-, RII/FC; antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT 155215-87-5, Jun kinase
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT 217308-10-6
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)
IT 50-23-7, Hydrocortisone 54-85-3, Isoniazid 59-67-6, Niacin, biological studies 64-86-8, Colchicine 107-35-7, Taurine 518-34-3, Tetrandrine

1028-33-7, Pentifylline 1405-86-3, Glycyrrhizin 6493-05-6, Pentoxifylline 6493-06-7 10102-43-9, Nitric oxide, biological studies 53179-13-8, Pirfenidone 55242-55-2, Propentofylline 55837-20-2, Halofuginone 62571-86-2, Captopril 75847-73-3, Enalapril 80288-49-9, Furafylline 83150-76-9, Octreotide 85721-33-1, Ciprofloxacin 91161-71-6, Terbinafine 114798-26-4, Losartan **119290-87-8**, Acanthoic acid 120210-48-2, Tenidap
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT 50-88-4, Tritiated thymidine, biological studies 42459-79-0
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)

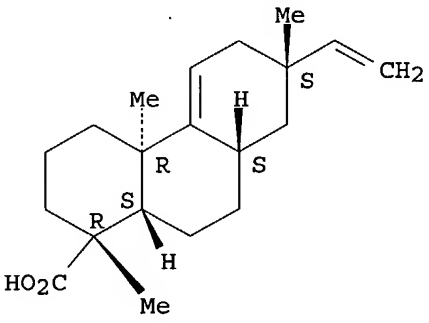
IT 330196-64-0, Cytochrome p 450 1A2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT 9015-82-1, Angiotensin converting enzyme
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; antisense oligonucleotide prepns. for treating fibroproliferative diseases)

IT **119290-87-8**, Acanthoic acid
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(antisense oligonucleotide prepns. for treating fibroproliferative diseases)

RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

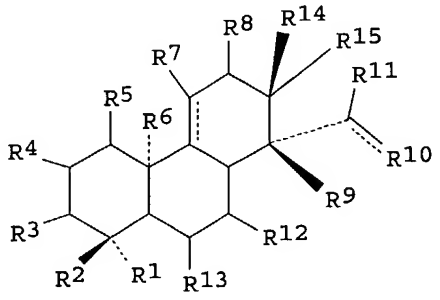


L50 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:861637 HCAPLUS
DN 134:5057
ED Entered STN: 08 Dec 2000
TI Novel interleukin-1 and tumor necrosis factor-a modulators, syntheses of said modulators and methods of using said modulators
IN **Palladino, Michael; Theodorakis, Emmanuel A.**
PA Nereus Pharmaceuticals, Inc., USA; Regents of the University of California
SO PCT Int. Appl., 98 pp.

CODEN: PIXXD2
DT **Patent**
LA English
IC ICM C07C061-35
ICS C07C061-29; C07C069-753; C07C069-757; C07C069-007; C07C069-00; C07C033-14; C07C013-60; A61K031-22; A61K031-215; A61K031-19; A61K031-045; A61K031-015
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): **1**
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000073253	A1	20001207	WO 2000-US13202	20000512 <--
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1178952	A1	20020213	EP 2000-932408	20000512 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000011522	A	20020604	BR 2000-11522	20000512 <--
	JP 2003500464	T2	20030107	JP 2000-621320	20000512 <--
	ZA 2001010246	A	20030313	ZA 2001-10246	20011213 <--
PRAI	US 1999-134295P	P	19990514 <--		
	US 2000-186853P	P	20000303		
	WO 2000-US13202	W	20000512		

OS CASREACT 134:5057; MARPAT 134:5057
GI



I

AB Syntheses of diterpenes (I) [R1 = H, halogen, CO2H, C1-C12 carboxylic acid, C1-C12 acyl halide, C1-C12 ester, C1-C12 secondary amine, C1-C12 tertiary amide, C1-C12 alc., C1-C12 ether, C1-C12 (un)substituted alkyl, C2-C12 (un)substituted alkenyl, C5-C12 aryl; R2, R9 sep. = H, halogen, C1-C12 (un)substituted alkyl, C2-C12 (un)substituted alkenyl, C2-C12 alkynyl, C1-C12 alc., C1-C12 acyl, C5-C12 aryl; R3, R4, R5, R7, R8, R11, R12, R13 sep. = H, halogen, C1-C12 (un)substituted alkyl, C2-C12 (un)substituted alkenyl, C2-C12 alkynyl, C5-C12 aryl; R6 = H, halogen, C1-C12 (un)substituted alkyl, C2-C12 (un)substituted alkenyl, C2-C12 alkynyl; R10 = H, halogen, CH2, C1-C6 (un)substituted alkyl, C2-C6 (un)substituted alkenyl, C1-C12 alc., C5-C12 aryl; R14, R15 sep. = H, halogen, CH2, C1-C6 (un)substituted alkyl, C2-C6 (un)substituted alkenyl,

C1-C6 alc., C5-C6 aryl] are disclosed and their prodrug esters and acid-addition salts, for use as interleukin-1 and tumor necrosis factor-a modulators in the treatment of various diseases. Thus, I (R1 = CO2H; R2, R6, R14 = Me; R3, R4, R5, R7, R8, R9, R12, R13 = H; R15 = CH=CH2; R11CH=R10 absent) (II) is prepared in 19 steps from 2-methyl-1,3-cyclohexanedione by addition of Me vinyl ketone, cyclization to naphthenedione, acetalization, carboxylation, alkynylation, reductive thiophenylation, dehydration, cyclization, reduction, oxidation, methylenation and saponification II inhibits SAC-induced TNF-α synthesis at 0.1 υg/mL.

ST diterpene prepn interleukin 1 modulator; tumor necrosis factor a modulator diterpene prepn

IT Cardiovascular system
(disease; syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT Ear
(otitis, otitis media; syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT Pleura
(pleurisy, tuberculous, rheumatoid; syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT Respiratory tract
(sinusitis; syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT Anti-inflammatory agents
Antidiabetic agents
Antitumor agents
Antiviral agents
Dermatitis
Transplant rejection
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT Interleukin 1
Tumor necrosis factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT **308795-78-0P 308795-79-1P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT **119290-87-8P**, NP 1302 **308795-85-9P 308795-86-0P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT **308795-84-8P**
RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT 74-88-4, Methyl iodide, reactions 78-85-3 78-94-4, Methyl vinyl ketone, reactions 603-35-0, Triphenylphosphine, reactions 1111-64-4, Lithium acetylide 1193-55-1 17640-15-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

IT 3487-44-3P 5073-65-4P 100348-93-4P **103462-23-3P**

117556-90-8P 187750-47-6P 287401-07-4P 287401-08-5P 287401-09-6P
287401-11-0P **287401-13-2P 287401-14-3P** 308795-75-7P
308795-76-8P **308795-77-9P** 308795-80-4P 308795-81-5P
308795-82-6P 308795-83-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

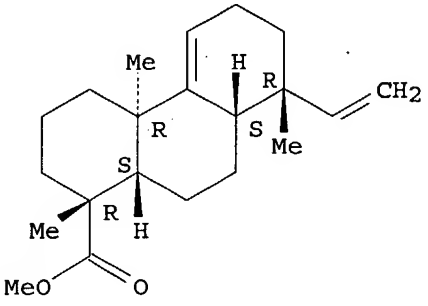
RE

(1) Fernanda, S; PHYTOCHEMISTRY 1986, V25(5), P1240
(2) Korea Institute Of Science And Technology; WO 9534300 A 1995 HCAPLUS
(3) Young, H; JOURNAL OF NATURAL PRODUCTS 1988, V51(6), P1080

IT **308795-78-0P 308795-79-1P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

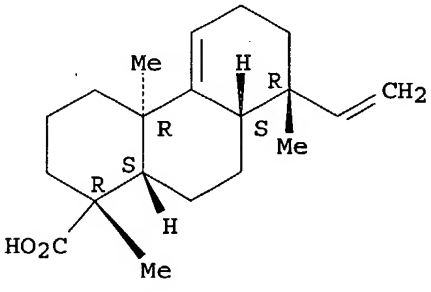
RN 308795-78-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 308795-79-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

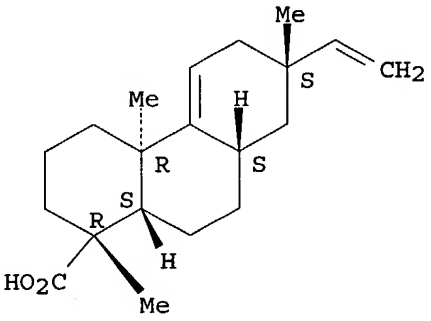


IT **119290-87-8P**, NP 1302 **308795-85-9P 308795-86-0P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES

(Uses)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

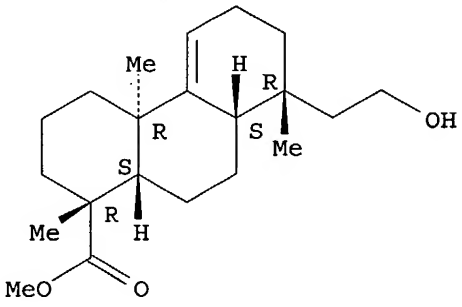
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



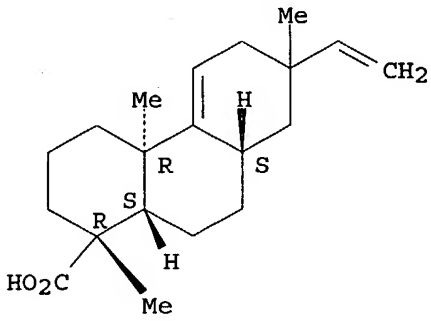
RN 308795-85-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(2-hydroxyethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 308795-86-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



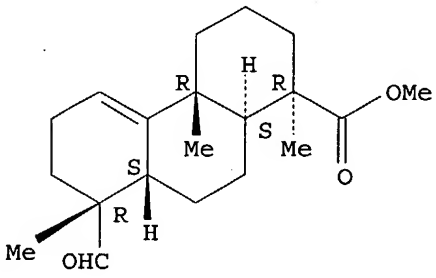
IT **308795-84-8P**

RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

RN 308795-84-8 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

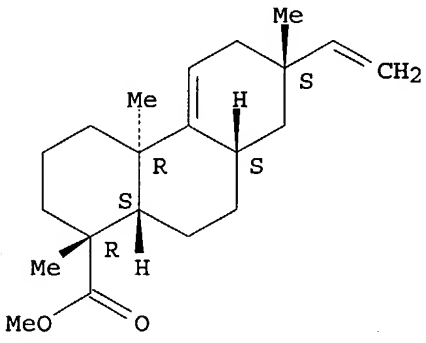


IT **103462-23-3P 287401-13-2P 287401-14-3P 308795-77-9P 308795-82-6P 308795-83-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses and methods of using diterpenes as interleukin-1 and tumor necrosis factor-a modulators)

RN 103462-23-3 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

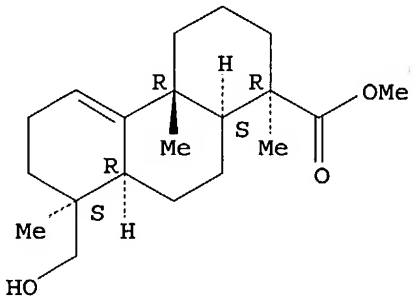
Absolute stereochemistry. Rotation (-).



RN 287401-13-2 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 287401-14-3 HCAPLUS
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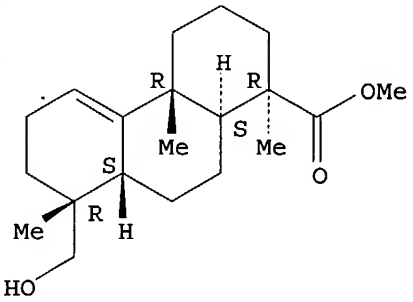
Absolute stereochemistry. Rotation (+).



RN 308795-77-9 HCAPLUS
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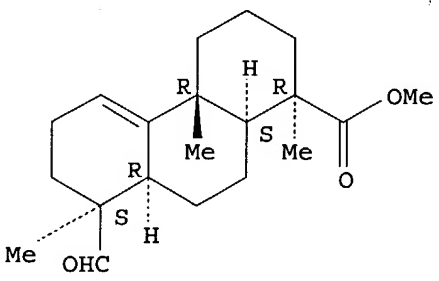
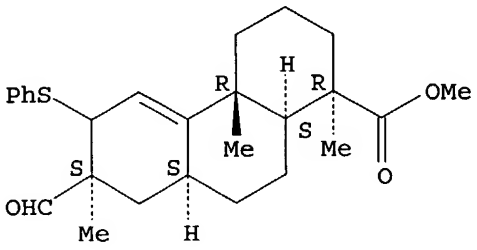
Absolute stereochemistry. Rotation (-).



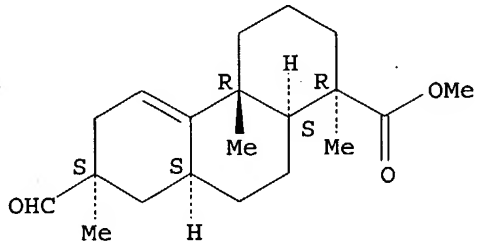
RN 308795-82-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-6-(phenylthio)-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 308795-83-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

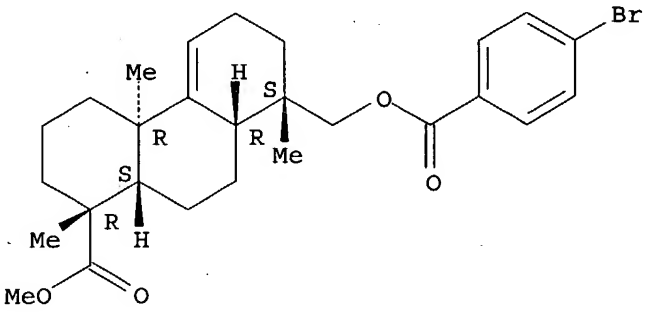


4/7

L50 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:402285 HCAPLUS
DN 133:150746
ED Entered STN: 18 Jun 2000
TI Stereoselective Synthesis of (-)-Acanthoic Acid
AU Ling, Taotao; Kramer, Bryan A.; **Palladino, Michael A.**; **Theodorakis, Emmanuel A.**
CS Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA, 92093-0358, USA
SO Organic Letters (2000), 2(14), 2073-2076
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
CC 30-20 (Terpenes and Terpenoids)
OS CASREACT 133:150746
AB The first stereoselective synthesis of (-)-acanthoic acid (I) has been designed and accomplished. Our synthetic plan departs from (-)-Wieland-Miesher ketone and calls upon a Diels-Alder cycloaddn. reaction for the construction of the C ring of I. The described synthesis confirms the proposed stereochem. of I and represents an efficient entry into an unexplored class of biol. active diterpenes.
ST acanthoic acid stereoselective synthesis Diels Alder
IT Diels-Alder reaction
Stereoselective synthesis
(stereoselective synthesis of (-)-acanthoic acid)
IT **287401-15-4P 287401-16-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; stereoselective synthesis of (-)-acanthoic acid)
IT 78-85-3 100348-93-4, (-)-Wieland-Miescher ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective synthesis of (-)-acanthoic acid)

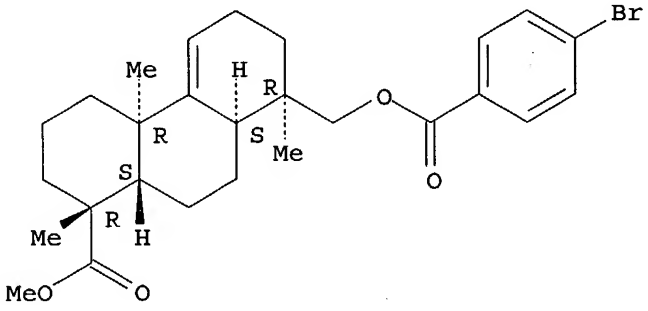
IT **103462-23-3P** 187750-47-6P 287401-06-3P 287401-07-4P
287401-08-5P 287401-09-6P 287401-10-9P 287401-11-0P
287401-12-1P 287401-13-2P 287401-14-3P
287401-17-6P 287478-47-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of (-)-acanthoic acid)
IT **119290-87-8P**, (-)-Acanthoic acid **187722-32-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of (-)-acanthoic acid)
RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Aggarwal, B; Human Cytokines Their Role in Disease and Therapy 1995
(2) Bennet, C; Tetrahedron 1967, V23, P927
(3) Beutler, B; Tumor Necrosis Factors The Molecules and their Emerging Role in Medicine 1992
(4) Buchschacher, P; Organic Syntheses 1990, V7, P368
(5) Coates, R; J Org Chem 1970, V35, P2597 HCAPLUS
(6) Coates, R; J Org Chem 1970, V35, P2601 HCAPLUS
(7) Cohen, T; J Org Chem 1982, V47, P4008
(8) Coisne, J; Bull Soc Chim Belg 1980, V89, P551 HCAPLUS
(9) Crabtree, S; Org Synth 1992, V70, P256 HCAPLUS
(10) Danishefsky, S; Angew Chem, Int Ed Engl 1994, V33, P853
(11) Das, J; Can J Chem 1984, V62, P1103 HCAPLUS
(12) Greengrass, C; J Chem Soc, Chem Commun 1985, P889 HCAPLUS
(13) Hopkins, P; J Org Chem 1978, V43, P1208 HCAPLUS
(14) Ireland, R; Tetrahedron Lett 1960, V25, P37
(15) Kang, H; Cellular Immunol 1996, V170, P212 HCAPLUS
(16) Kang, H; Mediators Inflammation 1988, V7, P257
(17) Kim, Y; J Nat Prod 1988, V51, P1080 HCAPLUS
(18) Kobuke, Y; J Am Chem Soc 1970, V92, P6548
(19) Kurzrock, R; Interleukins and Their Receptors 1995
(20) Lupin, E; Drugs 1998, V55, P613
(21) Mehta, G; J Am Chem Soc 1986, V108, P3443 HCAPLUS
(22) Newton, R; J Med Chem 1999, V42, P2295 HCAPLUS
(23) Oppolzer, W; Comprehensive Organic Synthesis 1991, P315
(24) Overman, L; J Am Chem Soc 1983, V105, P6335 HCAPLUS
(25) Perry, L; Medicinal Plants of East and Southeast Asia 1980
(26) Petrzilka, M; Synthesis 1981, P753 HCAPLUS
(27) Ruzicka, L; J Am Chem Soc 1948, V70, P2081
(28) Suh, Y; Arch Pharm Res 1995, V18, P217 HCAPLUS
(29) Suh, Y; Synth Commun 1997, V27, P587 HCAPLUS
(30) Szekanecz, Z; Clin Pharmacol 1998, V12, P377 MEDLINE
(31) Thorpe, R; Cytokines 1998
(32) Trost, B; J Am Chem Soc 1977, V99, P8116 HCAPLUS
(33) Trost, B; J Am Chem Soc 1980, V102, P7910 HCAPLUS
(34) Welch, S; J Am Chem Soc 1977, V99, P549 HCAPLUS
(35) Welch, S; J Org Chem 1977, V42, P2879 HCAPLUS
(36) Welch, S; Synth Commun 1973, V3, P29 HCAPLUS
(37) Wenkert, E; J Am Chem Soc 1959, V81, P688 HCAPLUS
(38) Wenkert, E; J Am Chem Soc 1972, V94, P4367 HCAPLUS
(39) Xiang, A; Angew Chem, Int Ed 1999, V38, P3089
(40) Xiang, A; J Org Chem 1998, V63, P6774 HCAPLUS
IT **287401-15-4P 287401-16-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; stereoselective synthesis of (-)-acanthoic acid)
RN 287401-15-4 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



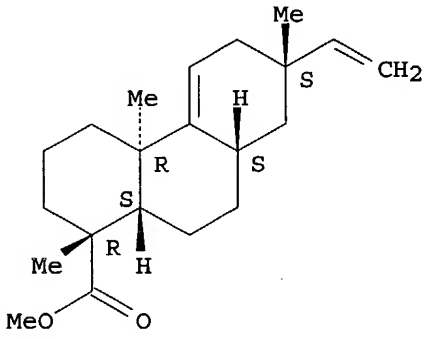
RN 287401-16-5 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-[[(4-bromobenzoyl)oxy]methyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



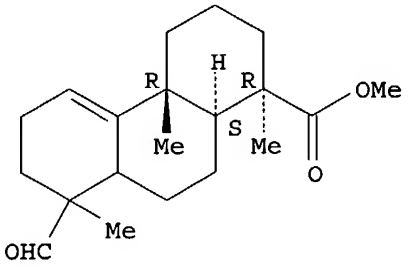
IT **103462-23-3P 287401-12-1P 287401-13-2P**
287401-14-3P 287401-17-6P 287478-47-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of (-)-acanthoic acid)
RN 103462-23-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



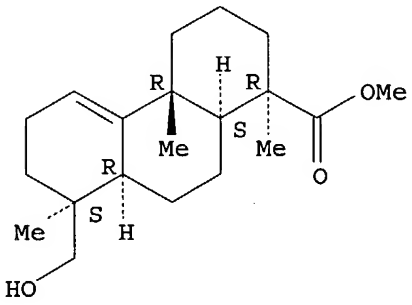
RN 287401-12-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 8-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



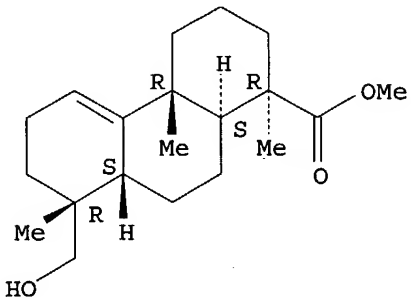
RN 287401-13-2 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8S,8aR,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



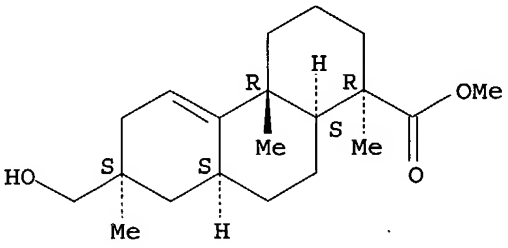
RN 287401-14-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-8-(hydroxymethyl)-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,8aS,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



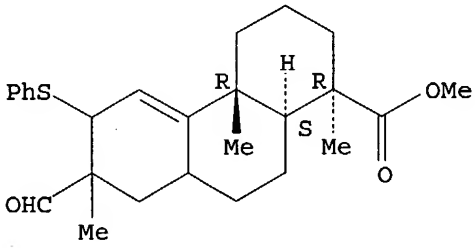
RN 287401-17-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(hydroxymethyl)-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



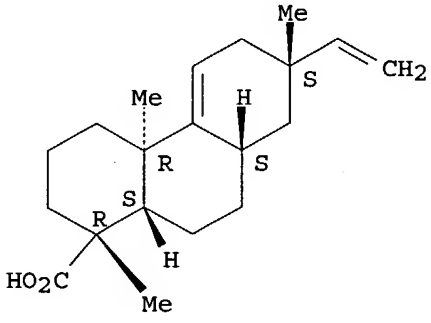
RN 287478-47-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-formyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-6-(phenylthio)-, methyl ester, (1R,4aR,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



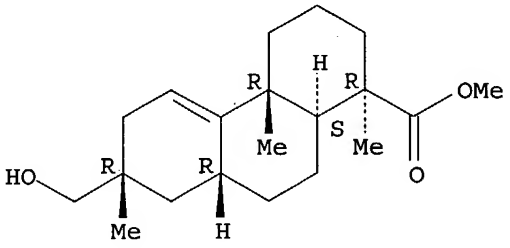
IT **119290-87-8P**, (-)-Acanthoic acid **187722-32-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of (-)-acanthoic acid)
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 187722-32-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(hydroxymethyl)-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7R,8aR,10aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:487259 HCAPLUS
DN 131:130145
ED Entered STN: 06 Aug 1999
TI Diterpene derivatives and anti-inflammatory analgesic agents comprising the same
IN Suh, Young Ger; Choi, Young Hoon; Lee, Hye Kyung; Kim, Young Ho; Park, Hyoung Sup
PA Sae Han Pharm. Co., Ltd., S. Korea
SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM C07C063-44
ICS C07C057-40; C07C233-00; C07C311-00; A61K031-19; A61K031-16
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): **1**, **63**
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9937600	A1	19990729	WO 1999-KR38	19990125 <--
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9921876	A1	19990809	AU 1999-21876	19990125 <--
	EP 1056710	A1	20001206	EP 1999-901968	19990125 <--
	EP 1056710	B1	20031210		
	R: CH, DE, ES, FR, GB, IT, LI				
	JP 2003502271	T2	20030121	JP 2000-528526	19990125 <--
	US 6593363	B1	20030715	US 2000-600774	20000915 <--
PRAI	KR 1998-2441	A	19980126 <--		
	WO 1999-KR38	W	19990125 <--		

OS MARPAT 131:130145
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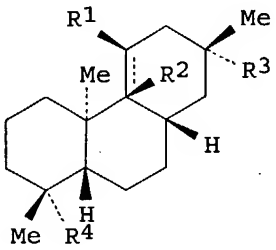


I

AB Title compds. I [R1, R2 = H, OH; or R1R2 = part of a ring; R3 = hydroxyethyl, methoxyethyl, acetoxyethyl, methoxymethoxyethyl, methoxyethoxymethoxyethyl, methoxyiminoethyl, isoxazolinyl; R4 = CH2OH, CH2COOH, carboxyvinyl, carboxyethyl, etc.] are prepared as antiinflammatories. Thus, (-)-pimara-9(11),15-diene-4-carboxylic acid was reduced with LiAlH4 to give 4-(hydroxymethyl)-(-)-pimara-9(11),15-diene. In an in vitro study, this had an IC50 of >2000 μM against PGE2 synthesis. Antiinflammatory compns. containing I are described.

ST diterpene deriv prepn antiinflammatory; pimaradiene deriv prepn antiinflammatory

IT Diterpenes
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(podocarpane; preparation of antiinflammatory diterpene derivs.)

IT Analgesics
Anti-inflammatory agents
(preparation of antiinflammatory diterpene derivs.)

IT 825-86-5P **103462-24-4P 233749-77-4P**
233749-78-5P 233749-79-6P 233749-80-9P
233749-81-0P 233749-83-2P 233749-84-3P
233749-85-4P 233749-90-1P 233749-92-3P
233749-93-4P **233749-97-8P 233749-99-0P**
233750-01-1P 233750-02-2P 233750-03-3P
233750-05-5P 233750-06-6P 233750-07-7P
233750-09-9P 233750-11-3P 233750-13-5P
233750-19-1P 233750-20-4P 233750-22-6P
233750-24-8P 233750-26-0P 233750-28-2P
233750-29-3P
RL: ADV (Adverse effect, including toxicity); **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of antiinflammatory diterpene derivs.)

IT **233749-82-1P 233749-86-5P 233749-87-6P**
233749-88-7P 233749-89-8P 233749-91-2P 233749-94-5P
233749-95-6P 233749-96-7P 233749-98-9P
233750-00-0P 233750-04-4P 233750-08-8P
233750-10-2P 233750-12-4P 233750-15-7P
233750-16-8P 233750-17-9P 233750-18-0P
233750-21-5P 233750-23-7P 233750-25-9P
233750-27-1P 233750-32-8P
RL: ADV (Adverse effect, including toxicity); **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiinflammatory diterpene derivs.)

IT 74-89-5, Methylamine, reactions 98-61-3, Pipsyl chloride 107-29-9, Acetaldoxime 593-56-6, Methoxylamine hydrochloride 867-13-0, Triethyl phosphonoacetate 2916-68-9, 2-(Trimethylsilyl)ethanol 3144-09-0, Methanesulfonamide 3970-21-6, 2-Methoxyethoxymethyl chloride 4009-98-7, (Methoxymethyl)triphenylphosphonium chloride 5470-11-1, Hydroxylamine hydrochloride 7803-57-8, Hydrazine monohydrate **119290-87-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of antiinflammatory diterpene derivs.)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

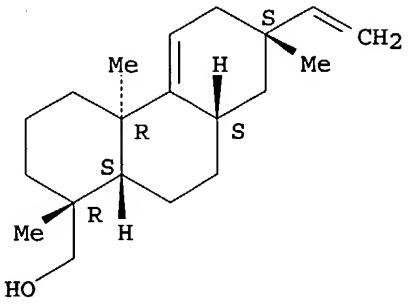
RE

(1) Anon; 1972, 15, P193 HCAPLUS
(2) Anon; 1991, 3, P408 HCAPLUS
(3) Anon; 1992, 11, P411 HCAPLUS
(4) Anon; 1997, 1, P594 HCAPLUS
(5) Chamy, C; Phytochemistry 1990, V29(9), P2943
(6) Chamy, C; Phytochemistry 1991, V30(10), P3365
(7) Cruz, F; Ouim Nora 1997, V20(3), P261 HCAPLUS
(8) Korea Institute Of Science And Technology; WO 9534300 A1 1995 HCAPLUS
(9) Morozkov, V; Ser Khim Nauk 1972, 1, P128 HCAPLUS

IT **103462-24-4P 233749-77-4P 233749-78-5P 233749-79-6P 233749-80-9P 233749-81-0P 233749-83-2P 233749-84-3P 233749-85-4P 233749-90-1P 233749-92-3P 233749-97-8P 233749-99-0P 233750-01-1P 233750-02-2P 233750-03-3P 233750-05-5P 233750-06-6P 233750-07-7P 233750-09-9P 233750-11-3P 233750-13-5P 233750-19-1P 233750-20-4P 233750-22-6P 233750-24-8P 233750-26-0P 233750-28-2P 233750-29-3P**
RL: ADV (Adverse effect, including toxicity); **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of antiinflammatory diterpene derivs.)

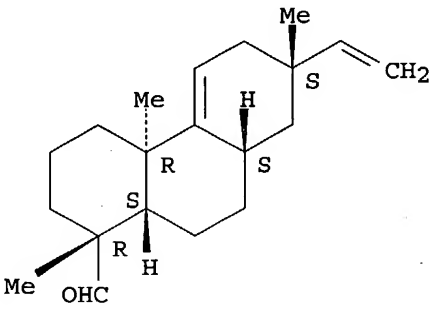
RN 103462-24-4 HCAPLUS
CN 1-Phenanthrenemethanol, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



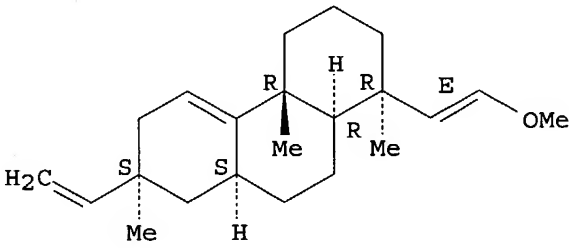
RN 233749-77-4 HCAPLUS
CN 1-Phenanthrenecarboxaldehyde, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



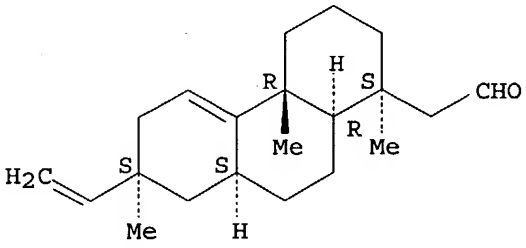
RN 233749-78-5 HCAPLUS
CN Phenanthrene, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1-[(1E)-2-methoxyethenyl]-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



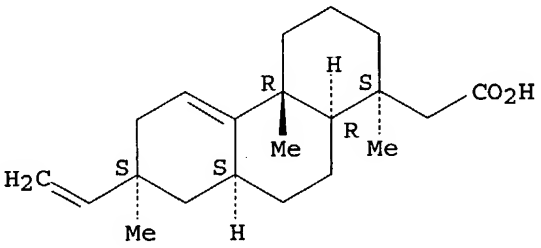
RN 233749-79-6 HCAPLUS
CN 1-Phenanthreneacetaldehyde, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



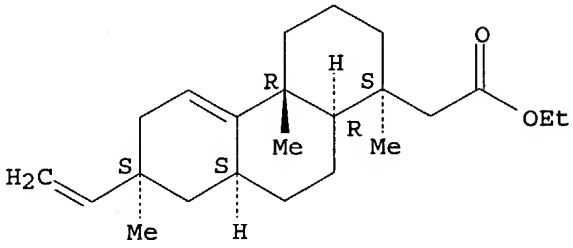
RN 233749-80-9 HCAPLUS
CN 1-Phenanthreneacetic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



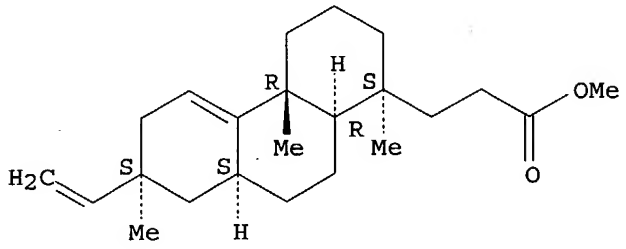
RN 233749-81-0 HCAPLUS
CN 1-Phenanthreneacetic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, ethyl ester, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



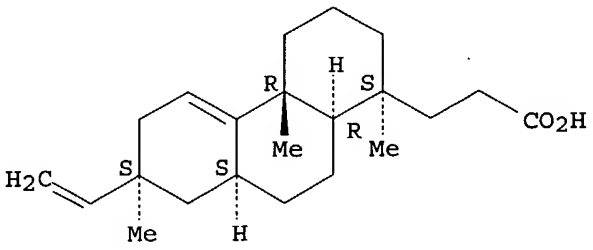
RN 233749-83-2 HCAPLUS
CN 1-Phenanthrenepropanoic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



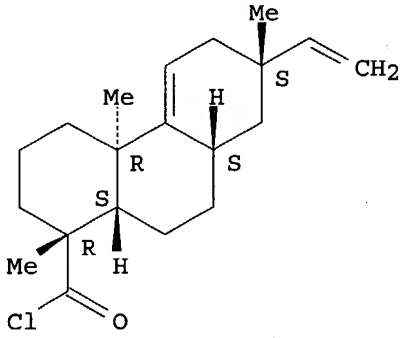
RN 233749-84-3 HCAPLUS
CN 1-Phenanthrenepropanoic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



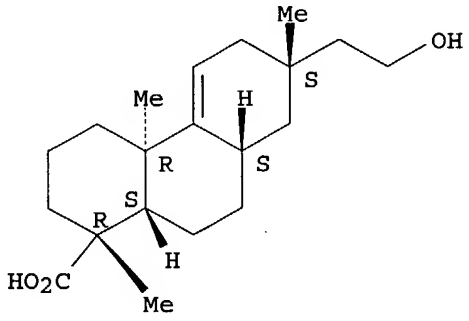
RN 233749-85-4 HCAPLUS
CN 1-Phenanthrenecarbonyl chloride, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



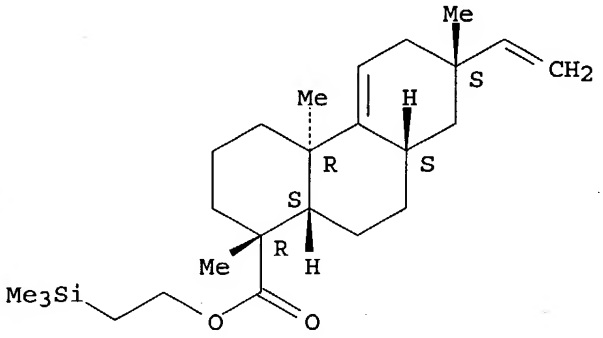
RN 233749-90-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(2-hydroxyethyl)-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



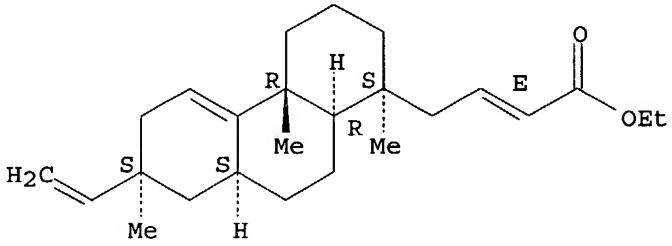
RN 233749-92-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



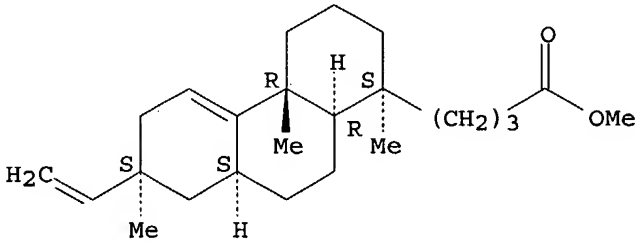
RN 233749-97-8 HCAPLUS
CN 2-Butenoic acid, 4-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



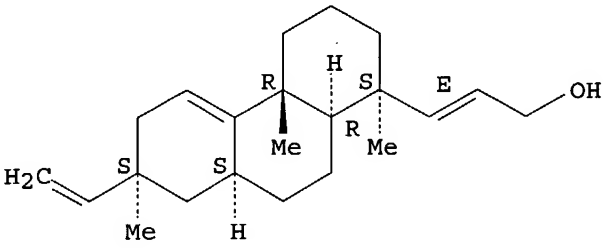
RN 233749-99-0 HCAPLUS
CN 1-Phenanthrenebutanoic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



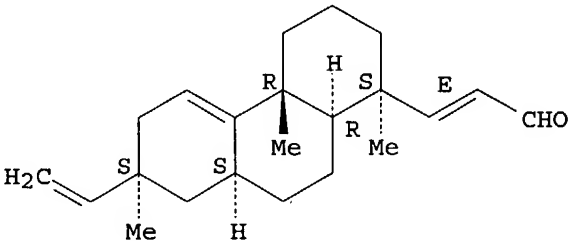
RN 233750-01-1 HCAPLUS
CN 2-Propen-1-ol, 3-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



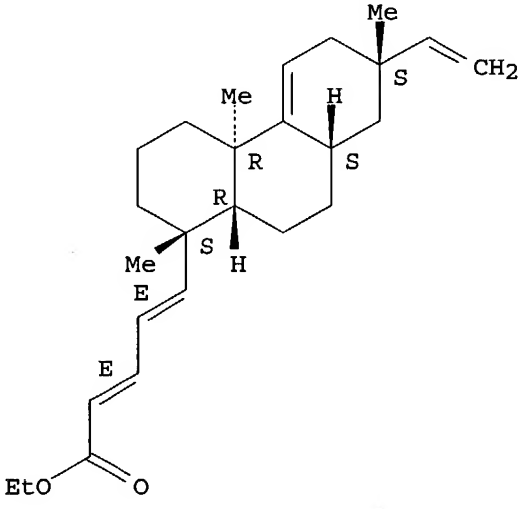
RN 233750-02-2 HCAPLUS
CN 2-Propenal, 3-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



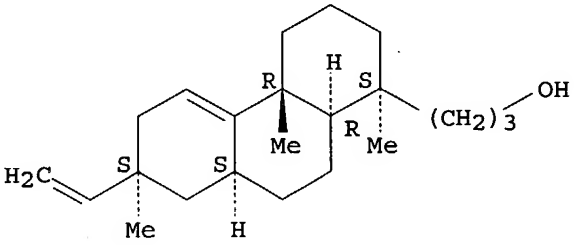
RN 233750-03-3 HCAPLUS
CN 2,4-Pentadienoic acid, 5-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, ethyl ester, (2E,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



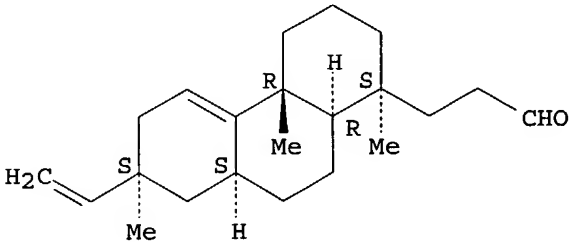
RN 233750-05-5 HCAPLUS
CN 1-Phenanthrenepropanol, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



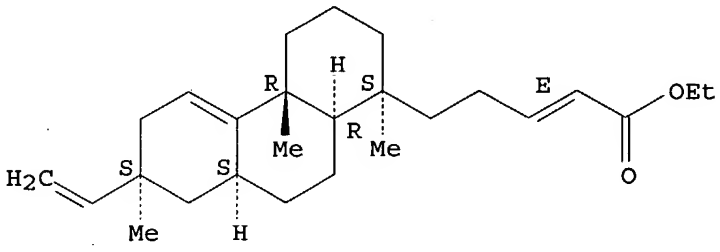
RN 233750-06-6 HCAPLUS
CN 1-Phenanthrenepropanal, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



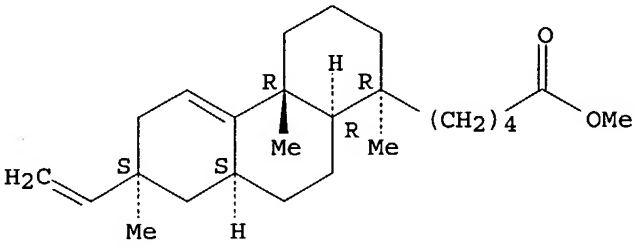
RN 233750-07-7 HCAPLUS
CN 2-Pentenoic acid, 5-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



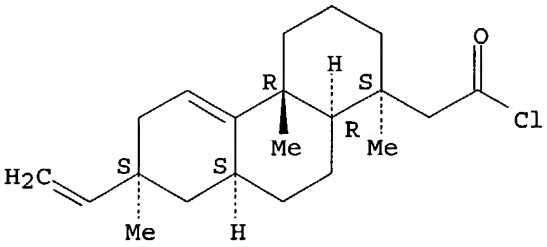
RN 233750-09-9 HCAPLUS
CN 1-Phenanthrenepentanoic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, (1R,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



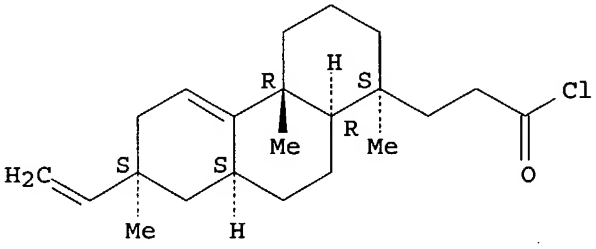
RN 233750-11-3 HCAPLUS
CN 1-Phenanthreneacetyl chloride, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



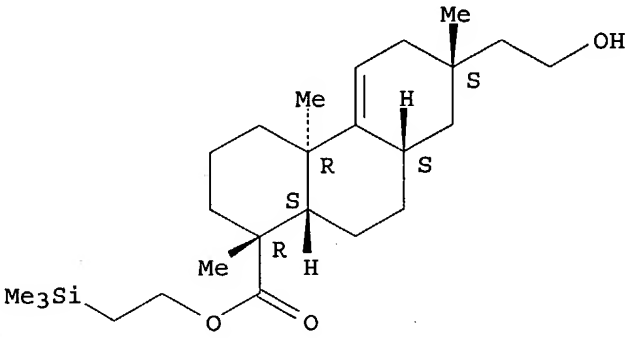
RN 233750-13-5 HCAPLUS
CN 1-Phenanthrenepropanoyl chloride, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



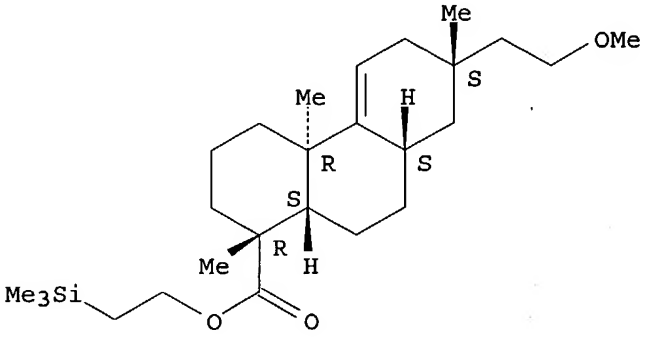
RN 233750-19-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(2-hydroxyethyl)-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



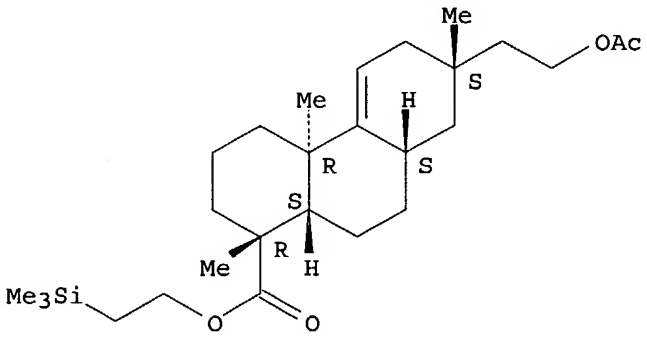
RN 233750-20-4 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(2-methoxyethyl)-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



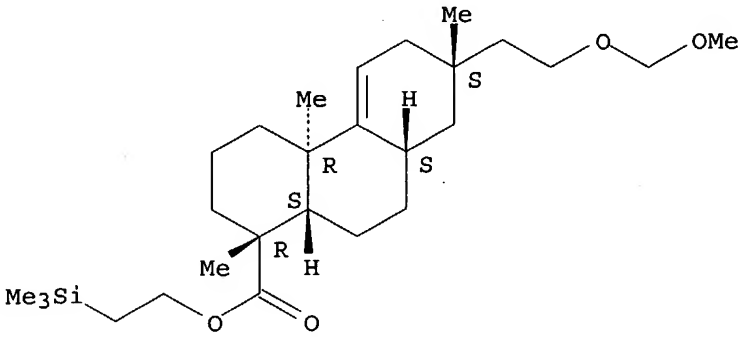
RN 233750-22-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-[2-(acetyloxy)ethyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



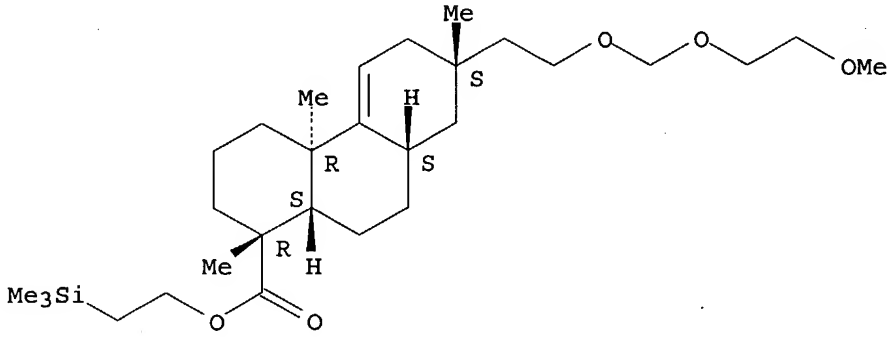
RN 233750-24-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-[2-(methoxymethoxy)ethyl]-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



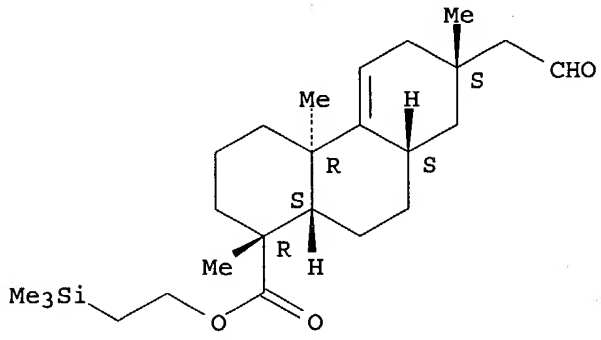
RN 233750-26-0 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-[2-[(2-methoxyethoxy)methoxy]ethyl]-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



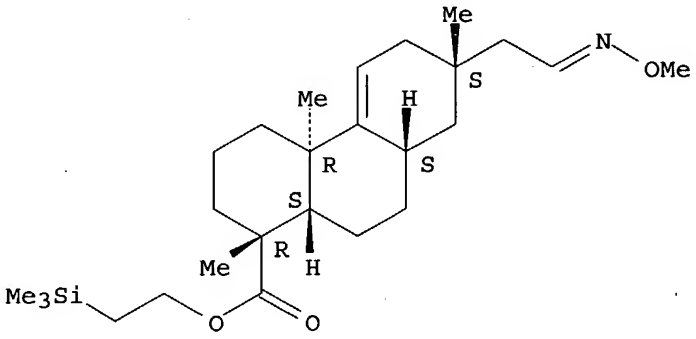
RN 233750-28-2 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-7-(2-oxoethyl)-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 233750-29-3 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-[2-(methoxyimino)ethyl]-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

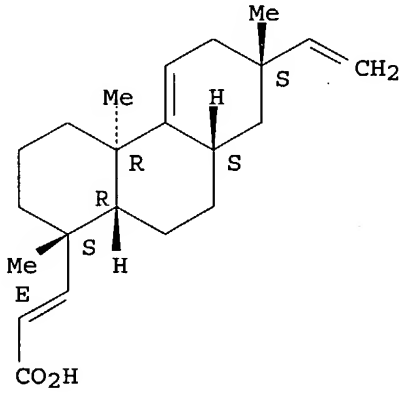
Absolute stereochemistry.
Double bond geometry unknown.



IT **233749-82-1P 233749-86-5P 233749-87-6P**
233749-88-7P 233749-89-8P 233749-95-6P
233749-96-7P 233749-98-9P 233750-00-0P
233750-04-4P 233750-08-8P 233750-10-2P
233750-12-4P 233750-15-7P 233750-16-8P
233750-17-9P 233750-18-0P 233750-21-5P
233750-23-7P 233750-25-9P 233750-27-1P
233750-32-8P
RL: ADV (Adverse effect, including toxicity); **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiinflammatory diterpene derivs.)

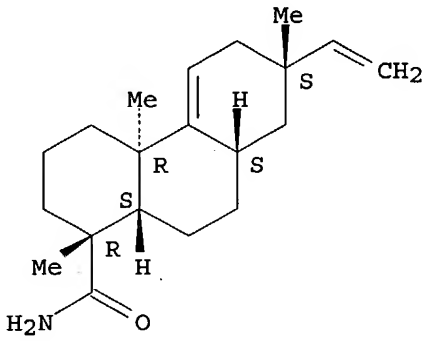
RN 233749-82-1 HCAPLUS
CN 2-Propenoic acid, 3-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



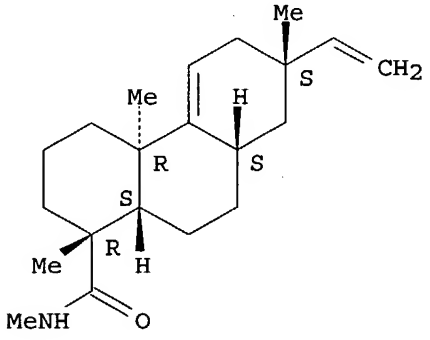
RN 233749-86-5 HCAPLUS
CN 1-Phenanthrenecarboxamide, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



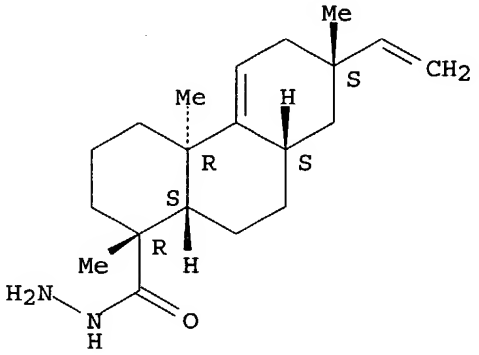
RN 233749-87-6 HCAPLUS
CN 1-Phenanthrenecarboxamide, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-N,1,4a,7-tetramethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



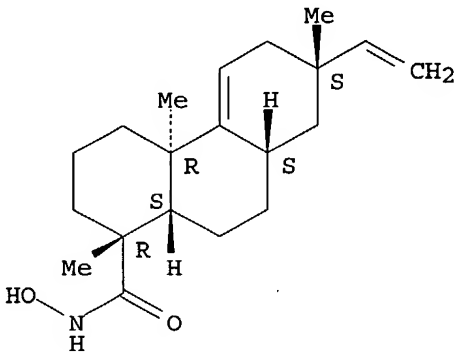
RN 233749-88-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, hydrazide, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



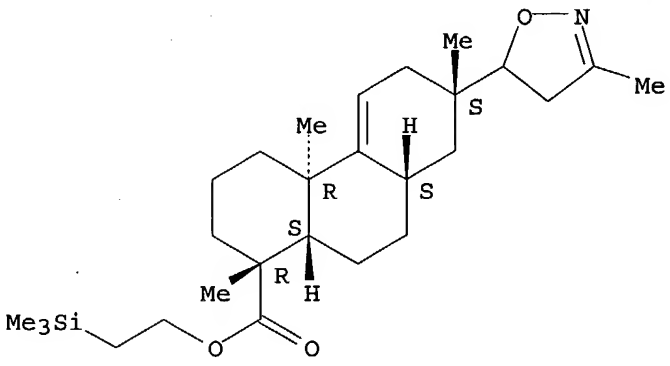
RN 233749-89-8 HCAPLUS
CN 1-Phenanthrenecarboxamide, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-N-hydroxy-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



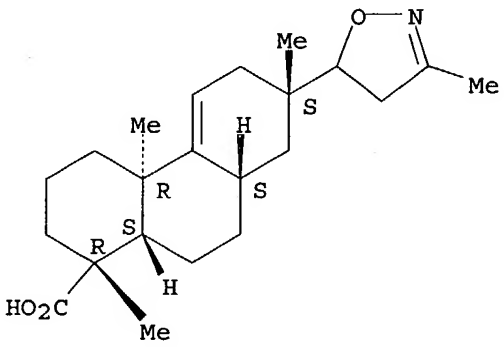
RN 233749-95-6 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-(4,5-dihydro-3-methyl-5-isoxazolyl)-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, 2-(trimethylsilyl)ethyl ester, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 233749-96-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-(4,5-dihydro-3-methyl-5-isoxazolyl)-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

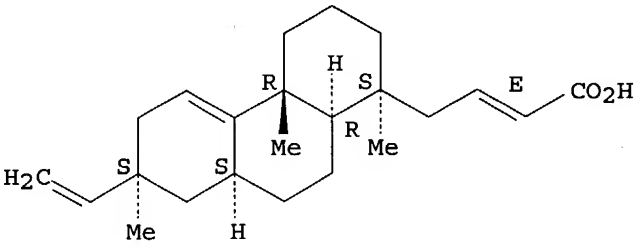
Absolute stereochemistry.



RN 233749-98-9 HCAPLUS
CN 2-Butenoic acid, 4-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-

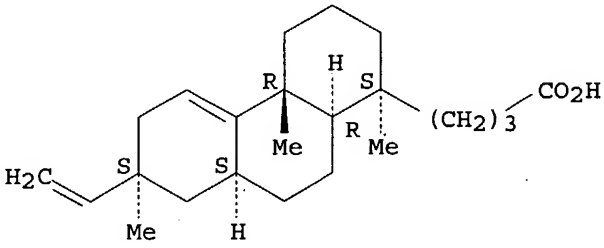
, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



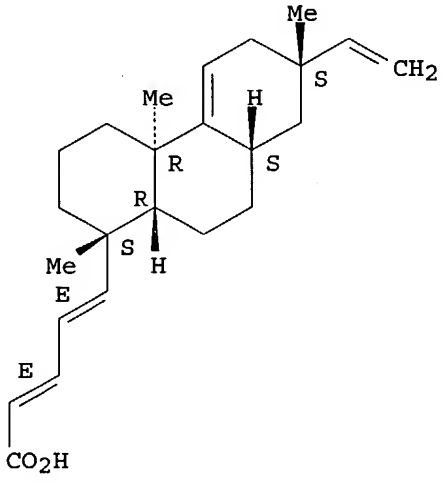
RN 233750-00-0 HCAPLUS
CN 1-Phenanthrenebutanoic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 233750-04-4 HCAPLUS
CN 2,4-Pentadienoic acid, 5-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, (2E,4E)- (9CI) (CA INDEX NAME)

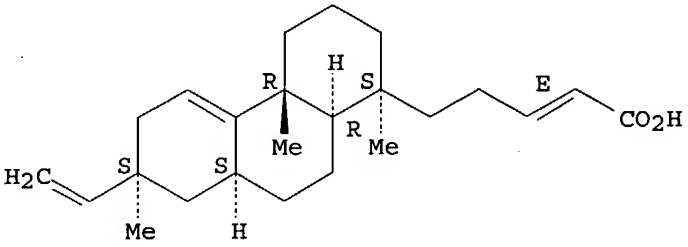
Absolute stereochemistry.
Double bond geometry as shown.



RN 233750-08-8 HCAPLUS
CN 2-Pentenoic acid, 5-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-

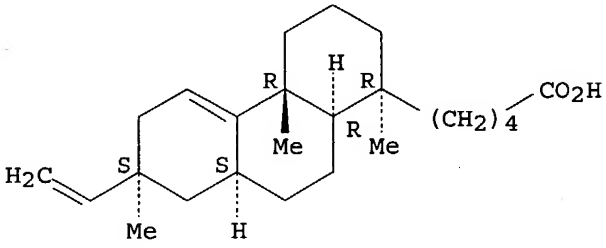
1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



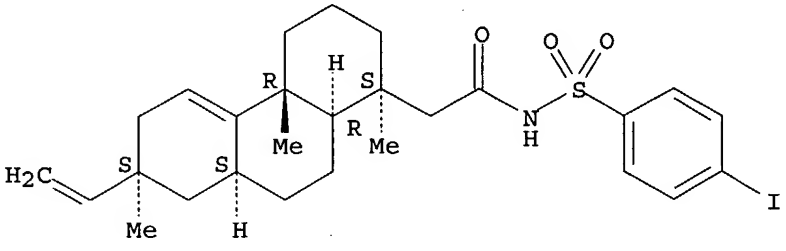
RN 233750-10-2 HCAPLUS
CN 1-Phenanthrenepentanoic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



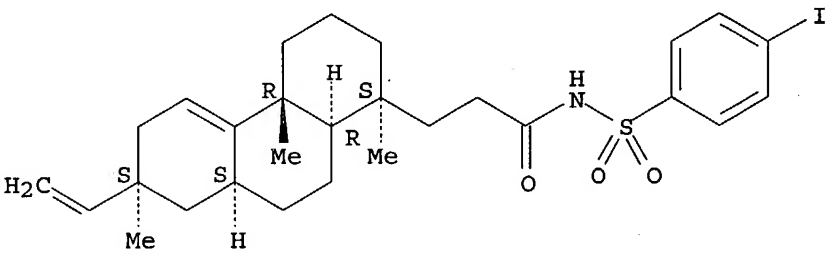
RN 233750-12-4 HCAPLUS
CN 1-Phenanthreneacetamide, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-N-[(4-iodophenyl)sulfonyl]-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



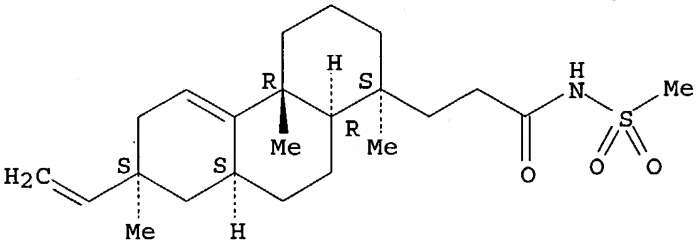
RN 233750-15-7 HCAPLUS
CN 1-Phenanthrenepropanamide, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-N-[(4-iodophenyl)sulfonyl]-1,4a,7-trimethyl-, (1S,4aR,7S,8aS,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



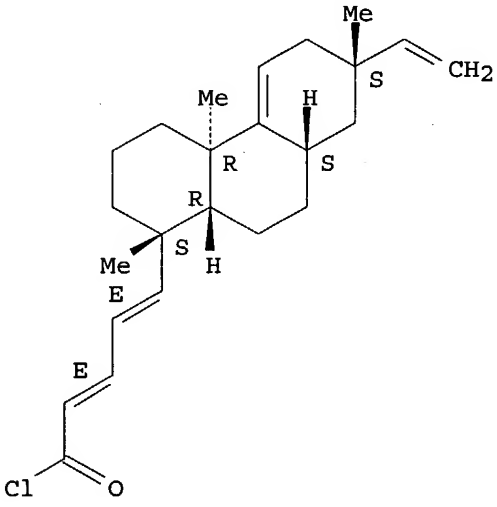
RN 233750-16-8 HCAPLUS
CN 1-Phenanthrenepropanamide, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-N-(methylsulfonyl)-, (1S,4aR,7S,8aS,10aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



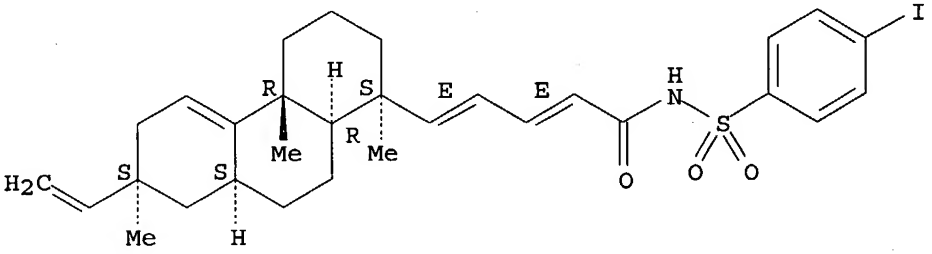
RN 233750-17-9 HCAPLUS
CN 2,4-Pentadienoyl chloride, 5-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-, (2E,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



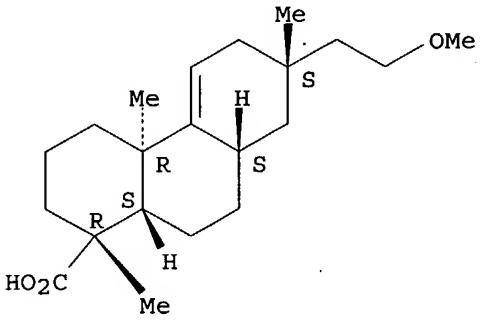
RN 233750-18-0 HCAPLUS
CN 2,4-Pentadienamide, 5-[(1S,4aR,7S,8aS,10aR)-7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-1-phenanthrenyl]-N-[(4-iodophenyl)sulfonyl]-, (2E,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



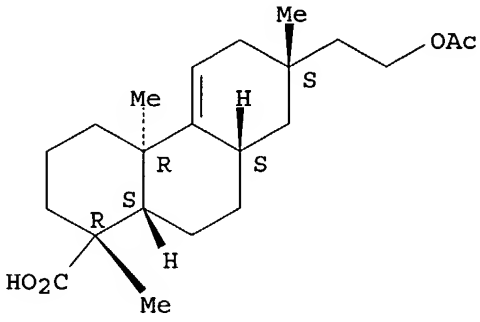
RN 233750-21-5 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-(2-methoxyethyl)-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



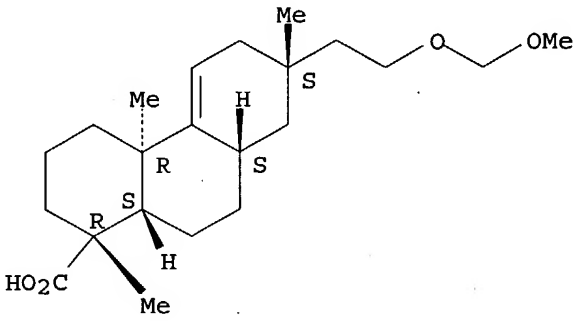
RN 233750-23-7 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-[2-(acetyloxy)ethyl]-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



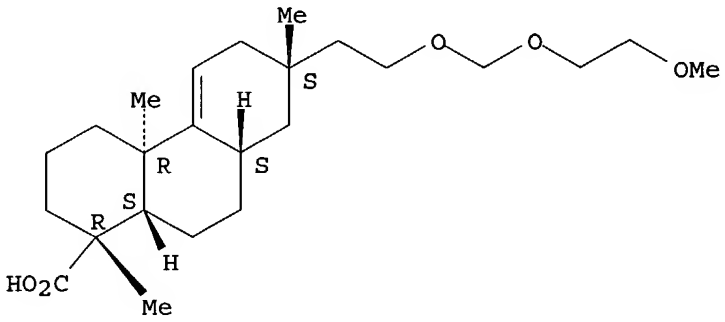
RN 233750-25-9 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-[2-(methoxymethoxy)ethyl]-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



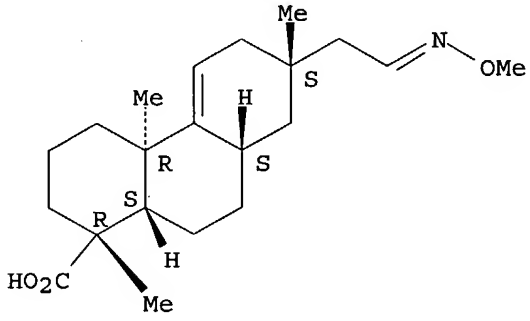
RN 233750-27-1 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-[2-[(2-methoxyethoxy)methoxy]ethyl]-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



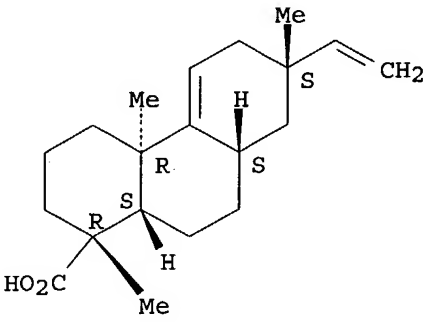
RN 233750-32-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-7-[2-(methoxyimino)ethyl]-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

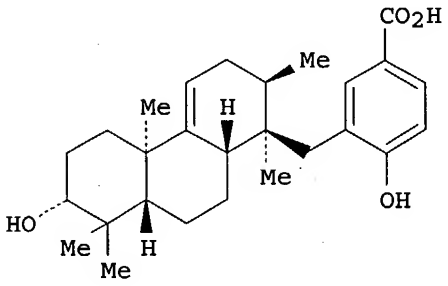


IT **119290-87-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of antiinflammatory diterpene derivs.)
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:140183 HCAPLUS
DN 130:293709
ED Entered STN: 05 Mar 1999
TI A Novel Extracellular Diterpenoid with Antibacterial Activity from the Cyanobacterium Nostoc commune
AU Jaki, Birgit; Orjala, Jimmy; Sticher, Otto
CS Department of Pharmacy, Swiss Federal Institute of Technology (ETH) Zurich, Zurich, CH-8057, Switz.
SO Journal of Natural Products (1999), 62(3), 502-503
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
CC 10-1 (Microbial, Algal, and Fungal Biochemistry)
Section cross-reference(s): 22, 30
GI



I

AB Noscomin (I), a novel extracellular diterpenoid metabolite, was isolated from the culture medium of the terrestrial cyanobacterium Nostoc commune Vaucher (EAWAG 122b) by means of bio-guided isolation. The structure was determined by spectroscopic methods, mainly NMR and mass spectrometry. Noscomin exhibited antibacterial activity against Bacillus cereus, Staphylococcus epidermidis, and Escherichia coli.
ST noscomin isolation mol structure Nostoc commune; diterpene noscomin isolation structure Nostoc; configuration noscomin isolation structure Nostoc; antibacterial activity noscomin isolation structure Nostoc
IT Antibacterial agents
Nostoc commune
(isolation and mol. structure of noscomin, a novel extracellular diterpenoid metabolite from the culture medium of the terrestrial cyanobacterium Nostoc commune)
IT Diterpenes

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and mol. structure of noscomin, a novel extracellular diterpenoid metabolite from the culture medium of the terrestrial cyanobacterium Nostoc commune)

IT New natural products
(noscomin (diterpene))

IT Configuration
Molecular structure, natural product
(of noscomin, a novel extracellular diterpenoid metabolite from the culture medium of the terrestrial cyanobacterium Nostoc commune)

IT **223414-56-0P**, Noscomin
RL: **BAC (Biological activity or effector, except adverse)**; BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and mol. structure of noscomin, a novel extracellular diterpenoid metabolite from the culture medium of the terrestrial cyanobacterium Nostoc commune)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

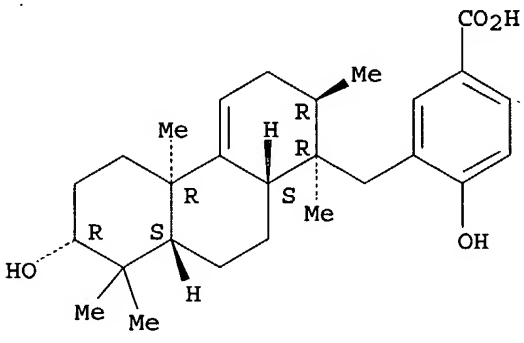
(1) Hughes, E; Can J Microbiol 1958, V4, P225 MEDLINE
(2) Moore, R; J Am Chem Soc 1984, V106, P6456 HCAPLUS
(3) Moore, R; J Org Chem 1987, V52, P1036 HCAPLUS
(4) Namikoshi, M; J Appl Phycol 1994, V6, P151
(5) Prinsep, M; J Nat Prod 1996, V59, P786 HCAPLUS
(6) Rios, J; J Ethnopharmacol 1988, V23, P127 HCAPLUS
(7) Schwartz, R; J Org Chem 1987, V52, P3704 HCAPLUS
(8) Simonin, P; Tetrahedron Lett 1992, V33, P3629 HCAPLUS
(9) Smitka, T; J Org Chem 1992, V57, P857 HCAPLUS
(10) Stratmann, K; J Am Chem Soc 1994, V116, P9935 HCAPLUS

IT **223414-56-0P**, Noscomin
RL: **BAC (Biological activity or effector, except adverse)**; BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and mol. structure of noscomin, a novel extracellular diterpenoid metabolite from the culture medium of the terrestrial cyanobacterium Nostoc commune)

RN 223414-56-0 HCAPLUS

CN Benzoic acid, 3-[[(1R,2R,4bR,7R,8aS,10aS)-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-1,2,4b,8,8-pentamethyl-1-phenanthrenyl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L50 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:637573 HCAPLUS
DN 130:47234
ED Entered STN: 09 Oct 1998
TI Effects of acanthoic acid on TNF-α gene expression and haptoglobin synthesis
AU Kang, H-S.; Song, H. K.; Lee, J-J.; Pyun, K-H.; Choi, I.
CS Immune Cell Signal Transduction Research Unit and Natural Product Biosynthesis Research Unit Korea Research Institute of Bioscience and Biotechnology, Taejon, 305-600, S. Korea
SO Mediators of Inflammation (**1998**), 7(4), 257-259
CODEN: MNFLEF; ISSN: 0962-9351
PB Carfax Publishing Ltd.
DT Journal
LA English
CC 1-7 (**Pharmacology**)
AB Tumor necrosis factor-α (TNF-α) is a major pro-inflammatory cytokine inducing the synthesis and release of many inflammatory mediators. It is involved in immune regulation, autoimmune diseases, and inflammation. Our previous study demonstrated that acanthoic acid, (-)-pimara-9(11), 15-dien-19-oic acid, a pimaradiene diterpene isolated from Acanthopanax koreanum, inhibited TNF-α production To extend our understanding of inhibitory effects of acanthoic acid on TNF-α production, its effects on TNF-α gene expression was tested. Based on the results from RT-PCR and promoter anal. of TNF-α, it was found that acanthoic acid suppressed TNF-α gene expression. But the same concentration of acanthoic acid had no effect on IL-6 gene expression. Haptoglobin is an acute phase protein which is induced by TNF-α. When liver cells were treated with acanthoic acid, haptoglobin synthesis was blocked by acanthoic acid. These data confirmed that acanthoic acid inhibited gene expression and biol. function of TNF-α.
ST acanthoic acid TNF gene expression haptoglobin; antiinflammatory acanthoic acid tumor necrosis factor
IT Anti-inflammatory agents
(acanthoic acid suppression of TNF-α gene expression and haptoglobin synthesis)
IT Haptoglobin
Tumor necrosis factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(acanthoic acid suppression of TNF-α gene expression and haptoglobin synthesis)
IT Gene
(expression; acanthoic acid suppression of TNF-α gene expression and haptoglobin synthesis)
IT **119290-87-8**, Acanthoic acid
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(acanthoic acid suppression of TNF-α gene expression and haptoglobin synthesis)
RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Cid, M; J Clin Invest 1993, V91, P977 HCAPLUS
(2) Dobryszycka, W; Eur J Clin Chem Clin Biochem 1997, V35, P647 HCAPLUS
(3) Douni, E; J Inflamm 1995, V45, P27
(4) Friedrichs, W; Biochem Biophys Res Commun 1995, V209, P250 HCAPLUS
(5) Kang, H; Cell Immunol 1996, V170, P212 HCAPLUS
(6) Kim, Y; J Nat Prod 1988, V51, P1080 HCAPLUS
(7) Lee, Y; PhD dissertation Seoul National University 1990
(8) Mullighan, C; J Immunol 1997, V159, P6236 HCAPLUS
(9) Nakagawa-Tosa, N; J Vet Med Sci 1995, V57, P219 HCAPLUS
(10) Rabinovitch, A; J Immunol 1996, V159, P6298

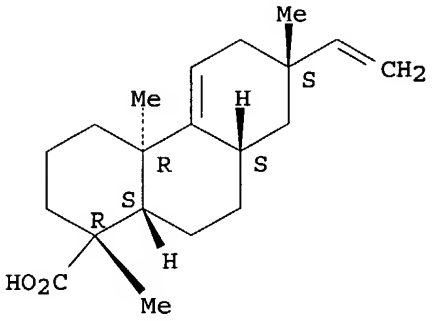
(11) Ross, S; J Immunol 1997, V159, P6253 HCAPLUS
(12) Ruddle, N; Curr Opin Immunol 1992, V4, P327 HCAPLUS
(13) Schmitz, H; Am J Physiol 1996, V271, P669

IT **119290-87-8**, Acanthoic acid
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(acanthoic acid suppression of TNF-α gene expression and haptoglobin synthesis)

RN 119290-87-8 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:496564 HCAPLUS
DN 129:230855
ED Entered STN: 11 Aug 1998
TI Synthetic Studies on Quassinoids: Total Synthesis and Biological Evaluation of (+)-Des-D-chaparrinone
AU Grieco, Paul A.; Speake, Jason D.
CS Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT, 59717, USA
SO Journal of Organic Chemistry (**1998**), 63(17), 5929-5936
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 30-15 (Terpenes and Terpenoids)
Section cross-reference(s): **1**, 75
OS CASREACT 129:230855
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A total synthesis of des-D-chaparrinone (I), which lacks the ring D δ-lactone of (-)-chaparrinone has been developed. The synthesis commences with the known, readily available tricyclic ketone (II). Elaboration of the configuration at C(5) followed by resolution of tricyclic ketone (III) (X = O) employing 2(R),3(R)-2,3-butanediol gave rise to III [X = (R,R)-OCH(βMe)CH(αMe)O]. Installation of the ring C functionality provided ketone (IV) which was transformed into tricyclic diketone (V). Introduction of the ring A functional groups afforded tricyclic enone (VI), which upon exposure to aluminum trichloride and

sodium iodide gave rise directly to (+)-des-D-chaparrinone I. Biol. studies revealed that (+)-I was devoid of any solid tumor activity.

ST chaparrinone des D synthesis antitumor; crystal structure configuration

IT Antitumor agents
(solid; total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

IT Crystal structure
(total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

IT 212965-54-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

IT 212953-69-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

IT 24347-58-8, (R,R)-(-)-2,3-Butanediol 212953-70-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

IT 135394-68-2P **212953-71-4P** 212953-72-5P 212953-73-6P
212953-74-7P 212953-75-8P 212953-76-9P 212953-77-0P 212953-78-1P
212953-79-2P 212953-80-5P 212953-81-6P 212953-82-7P 212953-83-8P
212953-84-9P 212965-41-8P 212965-44-1P 212965-46-3P 212965-49-6P
212965-51-0P 212965-56-5P 212965-58-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

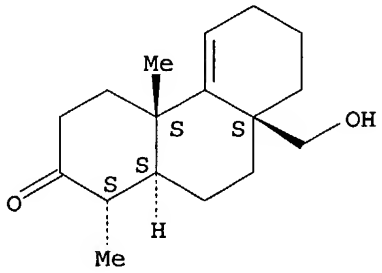
(1) Chamberlain, P; J Chem Soc (B) 1970, P1374 HCAPLUS
(2) Dess, D; J Am Chem Soc 1991, V113, P7277 HCAPLUS
(3) Grieco, P; J Am Chem Soc 1993, V115, P6078 HCAPLUS
(4) Grieco, P; J Am Chem Soc 1994, V116, P7606 HCAPLUS
(5) Hoveyda, A; Chem Rev 1993, V93, P1307 HCAPLUS
(6) Kupchan, S; J Med Chem 1976, V19, P1130 HCAPLUS
(7) Luche, J; J Am Chem Soc 1978, V100, P2226 HCAPLUS
(8) Moher, E; J Am Chem Soc 1992, V114, P2764 HCAPLUS
(9) Moher, E; J Org Chem 1998, V63, P3508 HCAPLUS
(10) Sharpless, K; Aldrichimica Acta 1979, V12, P63 HCAPLUS
(11) Snitman, D; J Org Chem 1978, V43, P4758 HCAPLUS
(12) Snitman, D; Synth Commun 1978, V8, P187 HCAPLUS
(13) Wall, M; Annu Rev Pharmacol Toxicol 1977, V17, P117 HCAPLUS

IT **212953-71-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis and biol. evaluation of (+)-des-D-chaparrinone)

RN 212953-71-4 HCAPLUS

CN 2(1H)-Phenanthrenone, 3,4,4a,6,7,8,8a,9,10,10a-decahydro-8a-(hydroxymethyl)-1,4a-dimethyl-, (1S,4aS,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:422982 HCAPLUS
DN 127:173799
ED Entered STN: 09 Jul 1997
TI Prenylated phenylpropenes from Coleonema pulchellum with antimicrobial activity
AU Brader, Gunter; Bacher, Markus; Hofer, Otmar; Greger, Harald
CS Comparative Phytochemistry Dep., Institute of Botany, University of Vienna, Vienna, A-1030, Austria
SO Phytochemistry (**1997**), 45(6), 1207-1212
CODEN: PYTCAS; ISSN: 0031-9422
PB Elsevier
DT Journal
LA English
CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 26
AB The lipophilic root extract of Coleonema pulchellum was analyzed and tested for antifungal and antibacterial activity. Eight previously undescribed prenyloxy and geranyloxy phenylpropenes, were isolated as major compds. together with the known evofolin-C as well as the lignans (±)-sesamin and (±)-prenylpiperitol, the diterpene (-)-pimara-9(11),15-dien-19-oic acid and the 2,4-decadienoic acid isobutylamide. All structures were established by spectroscopic evidence. From the new phenylpropenes, named evofolin-C-acetate, colenemol, colenemal, prenycol acetate, dehydroprenycol acetate, precolpuchol, colpuchol and colpuchol acetate, the dihydroxylated precolpuchol displayed the strongest antifungal and antibacterial activity against Cladosporium herbarum and Staphylococcus aureus, resp.
ST prenylated phenylpropene Coleonema antibacterial
IT New natural products
(colenemal (prenylated phenylpropene))
IT New natural products
(colenemol (prenylated phenylpropene))
IT New natural products
(colpuchol (prenylated phenylpropene))
IT Molecular structure, natural product
(of colenemal (prenylated phenylpropene))
IT Molecular structure, natural product
(of colenemol (prenylated phenylpropene))
IT Molecular structure, natural product
(of colpuchol (prenylated phenylpropene))
IT Molecular structure, natural product
(of precolpuchol (prenylated phenylpropene))
IT Molecular structure, natural product
(of prenycol acetate (prenylated phenylpropene))
IT New natural products
(precolpuchol (prenylated phenylpropene))
IT New natural products
(prenycol acetate (prenylated phenylpropene))
IT Antibacterial agents
Coleonema pulchellum
Fungicides
(prenylated phenylpropenes from Coleonema pulchellum with antimicrobial activity)
IT Cladosporium herbarum
Staphylococcus aureus
(prenylated phenylpropenes from Coleonema pulchellum with antimicrobial activity against)
IT **119290-87-8**
RL: **BAC (Biological activity or effector, except adverse)**; BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL

(Biological study); OCCU (Occurrence)
(antimicrobial activity of prenylated phenylpropenes and diterpene from Coleonema pulchellum)

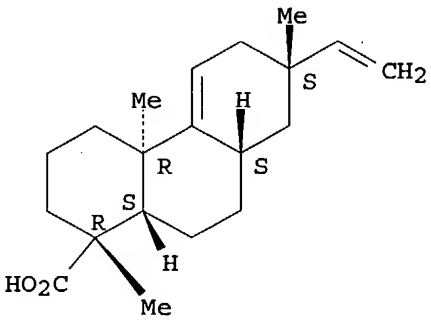
IT 109-26-2 81602-22-4, (±)-Sesamin 163634-05-7, Evofolin-C 194141-51-0
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(from Coleonema pulchellum)

IT 194141-48-5P, Evofolin-C-acetate 194141-49-6P, Dehydroprenycol acetate 194141-50-9P, Colpuchol acetate 194150-48-6P, Colenemol 194150-49-7P, Colenemal 194150-50-0P, Prenycol acetate 194150-51-1P, Precolpuchol 194150-52-2P, Colpuchol
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(prenylated phenylpropenes from Coleonema pulchellum with antimicrobial activity)

IT **119290-87-8**
RL: **BAC (Biological activity or effector, except adverse)**; BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(antimicrobial activity of prenylated phenylpropenes and diterpene from Coleonema pulchellum)

RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:378070 HCAPLUS
DN 125:75702
ED Entered STN: 29 Jun 1996
TI Suppression of interleukin-1 and tumor necrosis factor-α production by acanthoic acid, (-)-pimara-9(11),15-dien-19-oic acid, and its antifibrotic effects in vivo
AU Kang, Hyung-Sik; Kim, Young-Ho; Lee, Choong-Sik; Lee, Jung-Joon; Choi, Inpyo; Pyun, Kwang-Ho
CS Korea Res. Inst. Biosci. Biotechnology, Molecular Biomedicine Res. Group, Taejon, 305-600, S. Korea
SO Cellular Immunology (**1996**), 170(2), 212-221
CODEN: CLIMB8; ISSN: 0008-8749
PB Academic
DT Journal
LA English
CC 1-7 (**Pharmacology**)
AB Interleukin-1 (IL-1) and tumor necrosis factor-α (TNF-α) are

major proinflammatory cytokines inducing the synthesis and release of many inflammatory mediators. They are involved in immune regulation, autoimmune diseases, and inflammation. Acanthoic acid, (-)-pimara-9(11),15-dien-19-oic acid, is a pimaradiene diterpene isolated from the Korean medicinal plant, Acanthopanax koreanum. When human monocytes/macrophages stimulated with silica were treated with 0.1-10 μg/mL acanthoic acid, the production of Il-1 and TNF-α was inhibited ≤90%, but the production of interleukin-6 (IL-6) was not inhibited at all. At these concns., it had no cytotoxic effect on human monocytes/macrophages. It also suppressed the production of TNF-α by alveolar macrophages and lymphocytes stimulated with silica. In addition, acanthoic acid inhibited the release of superoxide anion and hydrogen peroxide from human monocytes/macrophages and neutrophils. To know the antifibrotic effects of acanthoic acid, its effects on fibroblast proliferation and collagen synthesis were tested. The proliferation of NIH3T3 cells was inhibited almost completely by the addition of the culture supernatants of human monocytes/macrophages treated with acanthoic acid, but not by the addition of acanthoic acid only. In vitro and in vivo treatment with acanthoic acid reduced collagen production by rat lung fibroblasts and lung tissue. Furthermore, acanthoic acid suppressed granuloma formation and fibrosis in the exptl. silicosis. Acanthoic acid reduced serum GOT and GPT in the rats with cirrhosis induced by CCl4, and it was effective in reducing hepatic fibrosis and nodular formation. Taken together, these data indicate that acanthoic acid has a potent anti-inflammatory and antifibrosis effect by reducing IL-1 and TNF-α production

ST acanthoate interleukin tumor necrosis factor antifibrotic

IT Fibrosis
Inflammation inhibitors
Macrophage
Monocyte
(suppression of interleukin-1 and tumor necrosis factor-α production in human monocytes/macrophages by acanthoic acid and antifibrotic and anti-inflammatory effects in vivo)

IT Lymphokines and Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(interleukin 1, suppression of interleukin-1 and tumor necrosis factor-α production in human monocytes/macrophages by acanthoic acid and antifibrotic and anti-inflammatory effects in vivo)

IT Lymphokines and Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(tumor necrosis factor-α, suppression of interleukin-1 and tumor necrosis factor-α production in human monocytes/macrophages by acanthoic acid and antifibrotic and anti-inflammatory effects in vivo)

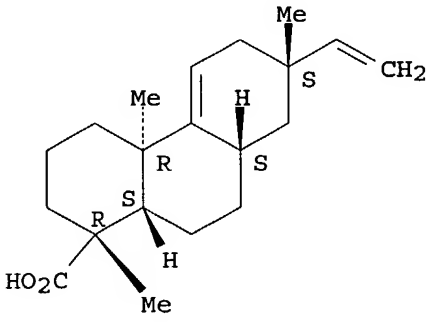
IT **119290-87-8**, Acanthoic acid
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(suppression of interleukin-1 and tumor necrosis factor-α production in human monocytes/macrophages by acanthoic acid and antifibrotic and anti-inflammatory effects in vivo)

IT **119290-87-8**, Acanthoic acid
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(suppression of interleukin-1 and tumor necrosis factor-α production in human monocytes/macrophages by acanthoic acid and antifibrotic and anti-inflammatory effects in vivo)

RN 119290-87-8 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L50 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:130879 HCAPLUS
DN 124:155966
ED Entered STN: 05 Mar 1996
TI Process for the preparation of acanthoic acid and pharmaceutical composition comprising same
IN Pyun, Kwang Ho; Choi, Inpyo; Kang, Hyung Sik; Lee, Jung Joon; Kim, Young Ho
PA Korea Institute of Science and Technology, S. Korea
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM A61K031-19
ICS A61K035-78
CC 63-4 (**Pharmaceuticals**)
Section cross-reference(s): **1**
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9534300	A1	19951221	WO 1995-KR74	19950607 <--
	W: CN, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 759751	A1	19970305	EP 1995-922773	19950607 <--
	R: AT, DE, FR, GB, IT				
	CN 1150758	A	19970528	CN 1995-193619	19950607 <--
	JP 10501549	T2	19980210	JP 1995-501958	19950607 <--
	US 5900434	A	19990504	US 1996-750459	19961206 <--
PRAI	KR 1994-13209		19940613 <--		
	WO 1995-KR74		19950607 <--		

AB Process for the preparation of (-)-pimara-9(11), 15-diene-19-oic acid (acanthoic acid) and pharmaceutical compns. comprising acanthoic acid useful for the treatment of diseases caused by an excessive production of interleukin-1 or tumor necrosis factor-α, are disclosed. Acanthoic acid was obtained by (1) extraction of well-dried root bark of Acanthopanax koreanum with MeOH, (2) partition of the extract with water/diethyl ether, and (3) purification of di-Et ether extract with silica gel column chromatog. and
TLC. Its inhibitory activities against production of IL-1 and TNF-α in human monocytes and macrophages, production of reactive oxygen species, proliferation of fibroblasts, and collagen synthesis, were studied.
ST acanthoic acid extn Acanthopanax immune disease
IT Acanthopanax koreanum

Cirrhosis
Inflammation
Sepsis and Septicemia
Silicosis
(extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Reactive oxygen species
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(production of; extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Fibroblast
(proliferation of; extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Collagens, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(synthesis of; extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Immunity
(disorder, extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Lymphokines and Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(interleukin 1, extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Lymphokines and Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(interleukin 6, extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Arthritis
(rheumatoid, extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT Lymphokines and Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(tumor necrosis factor-α, extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT **119290-87-8P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PUR (Purification or recovery); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

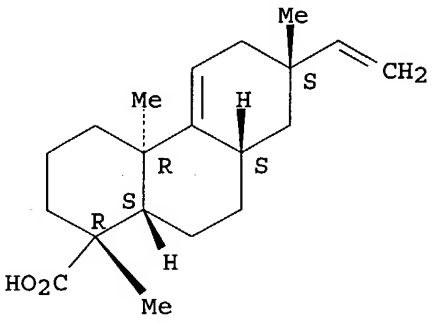
IT 9000-86-6, GPT 9000-97-9, GOT
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

IT **119290-87-8P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PUR (Purification or recovery); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(extraction of acanthoic acid from Acanthopanax koreanum and its use for treatment of immune diseases)

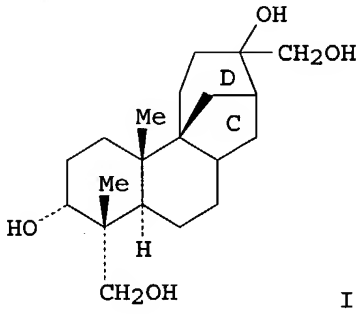
RN 119290-87-8 HCAPLUS
CN 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aR,7S,8aS,10aS)- (9CI) (CA INDEX

NAME)

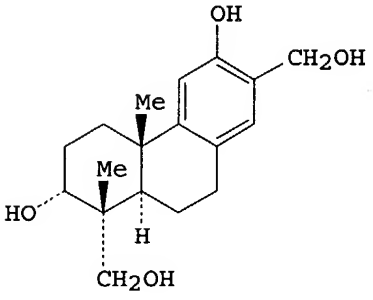
Absolute stereochemistry. Rotation (-).



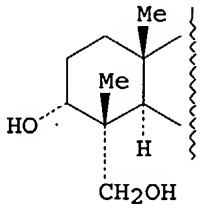
L50 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:134850 HCAPLUS
DN 120:134850
ED Entered STN: 19 Mar 1994
TI Isosteres of the DNA polymerase inhibitor aphidicolin as potential antiviral agents against human herpes viruses
AU Selwood, David L.; Challand, S. Richard; Champness, John N.; Gillam, Janet; Hibberd, Deborah K.; Jandu, K. Singh; Lowe, Denise; Pether, Michael; Selway, John; Trantor, George E.
CS Dep. Med. Chem., Wellcome Res. Lab., Beckenham/Kent, BR3 3BS, UK
SO Journal of Medicinal Chemistry (**1993**), 36(23), 3503-10
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): **1**
GI



I



II



III

AB A variety of isosteres of the DNA polymerase inhibitor aphidicolin (I) were synthesized as potential antiherpes agents. Modeling studies indicated that the bicyclooctane C, D rings of aphidicolin could be replaced by an aromatic moiety while maintaining the spatial arrangement of the hydroxyl group equivalent to the essential C18 hydroxyl group of aphidicolin. Of the racemic isosteres synthesized only II, the compound with the greatest structural similarity to aphidicolin, showed any significant antiviral activity in primary assays. An enantioselective synthesis of II was carried out and the 4aS isomer III was shown to account for the observed antiviral activity noted against herpes simplex virus 1 and human cytomegalovirus.

ST DNA polymerase inhibitor aphidocolin; isostere aphidocolin related virucide; podocarpatrienetetrol virucide; herpes aphidocolin related virucide

IT Virucides and Virustats
(aphidicolin isosteres as)

IT Virus, animal
(herpes simplex 1, aphidicolin isosteres for treatment of)

IT 917-64-6, Methylmagnesium iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with methoxytetralone)

IT 6836-19-7, 7-Methoxy-1-tetralone
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with methylmagnesium iodide)

IT 3886-69-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(as chiral auxiliary in synthesis of dimethylmethoxytetrahydrophenanthrenone)

IT 2627-86-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral auxiliary, in preparation of dimethylmethoxytetrahydrophenanthrenone)

IT 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation by, of podocarpatrienones)

IT 83999-81-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of, by Me cyanoformate)

IT 152694-61-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to amine)

IT 152564-84-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to methoxymethyltetralone)

IT 152564-85-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to phenanthrenone derivative)

IT 30021-91-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with osmium tetraoxide, diol from)

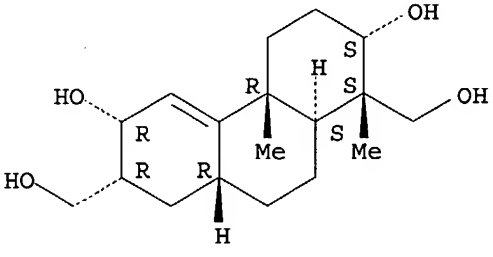
IT 152694-60-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with sodium thiocresolate)

IT 1204-23-5P 152564-64-2P 152694-59-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)

IT 152564-73-3P 152694-70-7P
RL: SPN (Synthetic preparation); PREP (Preparation)

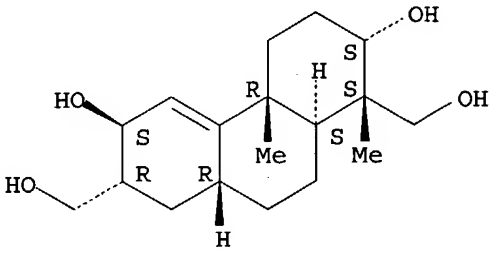
(preparation and reduction by DIBAL)
IT 152564-70-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 136087-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential formylation by Me cyanoformate and reduction of)
IT 152564-71-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and virucidal activity of)
IT 35011-71-3P 152564-65-3P 152564-66-4P 152564-67-5P 152564-68-6P
152564-69-7P 152564-72-2P **152564-74-4P 152564-75-5P**
152564-76-6P 152564-77-7P 152564-78-8P 152564-79-9P 152564-80-2P
152564-81-3P 152564-82-4P 152564-83-5P 152694-62-7P 152694-63-8P
152694-64-9P 152694-65-0P 152694-66-1P 152694-67-2P 152694-68-3P
152694-69-4P 152982-09-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 38966-21-1P, Aphidicolin
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isosteres of, virucidal activity in relation to)
IT 152694-58-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reaction with dichloromethyl ether, and sodium thiocresolate)
IT 4885-02-3, Dichloromethyl methyl ether
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aphidicolin-related compds.)
IT 1629-58-9, Ethyl vinyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylmethoxytetrahydromethylenone)
IT **152564-74-4P 152564-75-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 152564-74-4 HCAPLUS
CN 1,7-Phenanthrenedimethanol, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-2,6-dihydroxy-1,4a-dimethyl-, (1α,2α,4aβ,6α,7α,8aβ,10aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



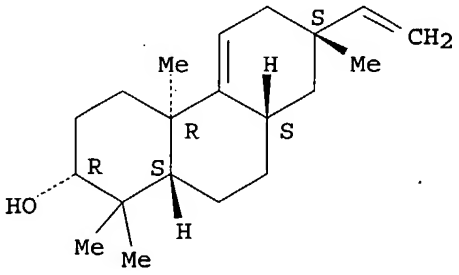
RN 152564-75-5 HCAPLUS
CN 1,7-Phenanthrenedimethanol, 1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-2,6-dihydroxy-1,4a-dimethyl-, (1α,2α,4aβ,6β,7α,8a.beta.,10aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



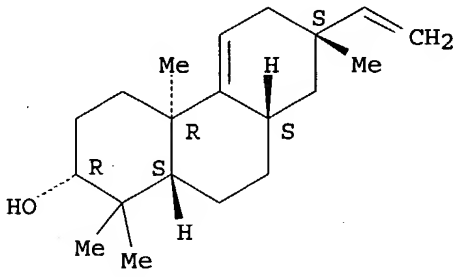
L50 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:531204 HCAPLUS
DN 119:131204
ED Entered STN: 02 Oct 1993
TI Nonspecific antispasmodic action of viguiepinol
AU Campos-Lozada, V.; Campos, E.; Guerrero, C.; Taboada, J.; Hernandec-Falcon, J; Fuentes-Pardo, B.
CS Fac. Med., Univ. Nac. Autono. Mexico, Mexico City, 04510, Mex.
SO Proceedings of the Western Pharmacology Society (**1993**), 36, 29-32
CODEN: PWPSA8; ISSN: 0083-8969
DT Journal
LA English
CC 1-8 (**Pharmacology**)
AB Previously the authors demonstrated a relaxant effect of viguiepinol (Vg) on aortic and ileal smooth muscle in vitro. A dose-response relationship was found between the magnitude of the relaxation and the Vg concentration The effects of Vg were reversed when the compound was withdrawn. These effects are equivalent to those found with similar compds. Vg is a diterpene (MW 288) extracted from the aerial portions of Viguiera pinnatilobata (Sch. Bip) Blake, a native plant distributed in southwest of Mexico and employed in infusions in traditional medicine. Due to the actions of Vg on two different kinds of smooth muscle and in accordance with the nonspecific actions of other diterpenes the present work was aimed at obtaining more evidence about its actions on uterine and bronchial smooth muscles. The muscles on which Vg acts have different membrane receptors responsible of the induction of their activity. The wide variety of muscles on which Vg is effective suggests that this diterpene acts through a nonspecific mechanism rather than via membrane receptors. The authors have no clear explanation for such a mechanism but changes in membrane fluidity, increase in membrane viscosity could be responsible. The relaxant actions provide an explanation for its employment in the traditional medicine and open the possibility of its use for clin. treatment. On the other hand it is necessary to obtain more information on the mechanisms of action of this diterpene.
ST viguiepinol antispasmodic
IT Muscle relaxants
(viguiepinol as)
IT **106386-94-1**, Viguiepinol
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antispasmodic activity of)
IT **106386-94-1**, Viguiepinol
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antispasmodic activity of)
RN 106386-94-1 HCAPLUS
CN 2-Phenanthrenol, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-, [2R-(2α,4aα,7α,8aβ,10aβ)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



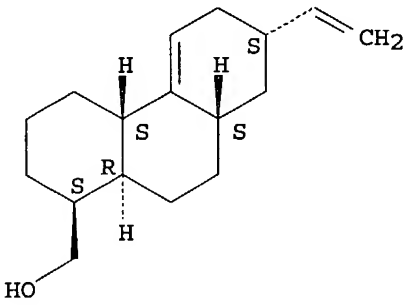
L50 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:647897 HCAPLUS
DN 115:247897
ED Entered STN: 14 Dec 1991
TI Relaxant effect of viguiepinol on smooth muscle in vitro
AU Hernandez-Falcon, J.; Taboada, J.; Guerrero, C.; Campos-Lozada, V.; Fernandezm, D.; Fuentes-Pardo, B.
CS Fac. Med., UNAM, Mexico City, 04510, Mex.
SO Proceedings of the Western Pharmacology Society (**1991**), 34, 199-203
CODEN: PWPSA8; ISSN: 0083-8969
DT Journal
LA English
CC 1-11 (**Pharmacology**)
AB The capacity of viguiepinol to relax the smooth muscle is greater in the rat ileum than in the rat aorta since, for the latter, doses of 1 + 10-2M must be used to detect a clear relaxant effect, whereas the effect upon the ileum can be obtained with doses as low as 1 + 10-7 M. However, comparing it with other substances having well established relaxant effects, viguiepinol is more potent than isoproterenol, which is a relaxant of the aorta and less potent than papaverine.
ST viguiepinol smooth muscle relaxant; ileum relaxant viguiepinol; aorta relaxant viguiepinol
IT Artery
(aorta, relaxation of, by viguiepinol)
IT Intestine
(ileum, relaxation of, by viguiepinol)
IT Muscle relaxants
(smooth, viguiepinol as, in aorta and ileum)
IT **106386-94-1**, Viguiepinol
RL: BIOL (Biological study)
(smooth muscle relaxant, in aorta and ileum)
IT **106386-94-1**, Viguiepinol
RL: BIOL (Biological study)
(smooth muscle relaxant, in aorta and ileum)
RN 106386-94-1 HCAPLUS
CN 2-Phenanthrenol, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-, [2R-(2α,4aα,7α,8aβ,10aβ)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

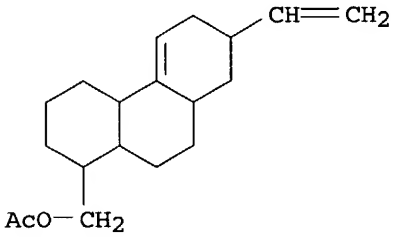


L50 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:578278 HCAPLUS
DN 105:178278
ED Entered STN: 15 Nov 1986
TI Studies on the constituents of Acanthopanax koreanum
AU Chung, Bo Sup; Kim, Young Ho
CS Coll. Pharm., Seoul Natl. Univ., Seoul, 151, S. Korea
SO Saengyak Hakhoechi (**1986**), 17(1), 62-6
CODEN: SYHJAM; ISSN: 0253-3073
DT Journal
LA English
CC 63-4 (**Pharmaceuticals**)
AB From the roots of A. koreanum, the exts. of which are used in treatment of rheumatism and paralysis and as sedatives, were isolated: lignans eleutheroside A [474-58-8], ariensin [81410-43-7], and syringin [118-34-3], a diterpenoid isopimara-9(11),15-dien-19-ol [**104697-02-1**], and a polyacetylene compound falcarindiol [55297-87-5]. The structures were determined by spectroscopic methods.
ST Acanthopanax lignan; isopimaradienol Acanthopanax; falcarindiol Acanthopanax
IT Acanthopanax koreanum
(lignans of)
IT Lignans
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Acanthopanax koreanum)
IT 118-34-3 474-58-8 55297-87-5 **104697-02-1**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Acanthopanax koreanum)
IT 81410-43-7
RL: BIOL (Biological study)
(of Acenthopanax koreanum)
IT 24562-96-7P 88010-45-1P **104672-10-8P** 104758-17-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **104697-02-1**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Acanthopanax koreanum)
RN 104697-02-1 HCAPLUS
CN 1-Phenanthrenemethanol, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-, [1S-(1α,4aα,7β,8aα,10aβ)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **104672-10-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 104672-10-8 HCAPLUS
CN 1-Phenanthrenemethanol, 7-ethenyl-1,2,3,4,4a,6,7,8,8a,9,10,10a-dodecahydro-, acetate, [1S-(1α,4aα,7β,8aα,10aβ)]- (9CI)
(CA INDEX NAME)



L50 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1965:91256 HCAPLUS
DN 62:91256
OREF 62:16347a-h,16348a-b
ED Entered STN: 22 Apr 2001
TI Steroids
PA Shionogi & Co., Ltd.
SO 20 pp.
DT **Patent**
LA English
IC C07C; C07D
CC 42 (Steroids)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	GB 984021		19650224	GB		<--
	DE 1203262			DE		
	US 3197485		1965	US		<--
PRAI	JP		19610719 <--			

GI For diagram(s), see printed CA Issue.
AB Preparation of pregnadienes with the general formula (I) was described, dl-17-Methoxy-D-homo-18-norandrosta-4,8,13,15,17-pentaen -3-one (3 g.) hydrogenated 160 min. at 25° over 0.6 g. 10% Pd-C in C6H6, EtOAc, and alc. gave 2.49 g. dl-17-methoxy-D-homo-18-nor-5β-androsta-8,13,15,17-tetraen-3-one (II), m. 82-5°(alc.). II (1 g.) in 10 ml. tetrahydrofuran (THF) treated with 2 g. tritert-butoxyaluminumlithium hydride in 10 ml. THF gave 855.8 mg. dl - 17-methoxy-D-homo-18-nor-5β-androsta-8,13,15,17-tetraen-3α-ol (III), m. 125-6° (Et2O).

III (3 g.) in 22 ml. dioxane, 46 ml. Et2O, and 38 ml. alc. added to 9 g. Li in 270 ml. liquid NH3 in 1.5 hrs., the mixture left 15 min. and worked up gave 3 g. of a residue. This residue refluxed with 125 ml. MeOH and 50 ml. 4N HCl and the product chromatographed on Al2O3 gave dl-3α-hydroxy-D-homo-18-nor-5β-androst-13(17a)-en-17-one (IV), m. 170-1° (alc.) and an isomer, m. 168-9° (Me2CO- Et2O). IV (400 mg.) in 5 ml. isopropenyl acetate refluxed 4 hrs. with 20 mg. p-MeC6H4SO3H gave 195.7 mg. dl-3α,17-di- acetoxy-D-homo-18-nor-5β-androsta-13,17-diene, m. 97-109° (Et2O-pentane). IV (68 mg.) similarly treated with isopropenyl acetate, the product in 137 ml. AcOH treated with collidine and 42 ml. 10% Br-AcOH, stirred 20 min. at 15-20°, the product extracted with Et2O, then treated with 10.5 g. LiBr in HCONMe2 and 10.5 g. Li2CO3, the mixture refluxed 40 min. after removal of Et2O, the product acetylated and chromatographed on Al2O3 gave 2.6 g. dl-3α-acetoxy-D-homo-18-nor-5β-androsta-11,13(17a)-dien-17-one (V), m. 149-51° (Et2O). V (290 mg.), 30 mg. C5H5N.HCl, 1.8 ml. Et orthoformate, 1.5 ml. alc., and 15 ml. C6H6 refluxed 3 hrs. gave 181.3 mg. dl-3α-acetoxy-17-ethoxy-D- homo-18-nor-5β-androsta-9(11),12,17-triene (VI), m. 118-22° to 130° (Et2O-pentane). VI (232 mg.) in 8 ml. AcOH and 8 ml. H2O warmed 15 min. at 90° gave 239.5 mg. crude 3α-acetoxy- D-homo-18-nor-5β-androsta-9(11),13(17a)-dien-17-one (VII). VII in 3 ml. THF added dropwise to 0.45 ml. AlEt3 and 0.52 ml. HCN in 7 ml. THF, the mixture left 2 hrs. at room temperature, and the product chromatographed on Al2O3 gave 120.8 mg. dl-3α- acetoxy-17-oxo-D-homo-5β-androst-9(11)-ene-18-nitrile (VIII), m. 249-51° (Me2CO-Et2O). V (2.6 g.) treated first with Et orthoformate and C5H5N.HCl and the crude product treated further with AlEt3 and HCN gave 1.53 g. VIII. VIII (85 mg.) in 12 ml. (CH2OH)2 refluxed 1 hr. at 4 mm. pressure at 75-80° with 4 mg. p-MeC6H4SO3H gave 78.6 mg. dl-3α- acetoxy-17,17-ethylenedioxy-D-homo-5β-androst-9(11)-ene-18- nitrile (IX), m. 251-2° (Me2CO-Et2O). IX (300 mg.) in 50 ml. THF added in 20 min. at 0° to 300 mg. LiAlH4 in 20 ml. THF, the mixture stirred 2 hrs. at room temperature, the product refluxed 7 hrs. with MeOH-NaOH in H2O, the crude product in 8.5 ml. triethylene glycol kept 1 hr. at 130-40° with 1.3 ml. 80% N2H4·H2O and 440 mg. KOH, then the temperature raised in 50 min. to 210°, maintained there for 3 hrs., and the product acetylated, and chromatographed on neutral Al2O3 gave 123 mg. dl-3α-acctoxy-17,17-ethylenedioxy-D-homo-5β-androst-9(11)- ene (X), m. 125-7° (Et2O-pentane). X (110 mg.) in 5 ml. AcOH and 2.5 ml. H2O heated and evaporated gave 88.9 mg. dl-3α-acetoxy- D-homo-5β-androst-9(11)-en-17-one (XI), m. 155-6.5° (Et2O- pentane). IX (1.1 g.) reduced with LiAlH4, the product treated with KOH and N2H4·H2O, the product in AcOH heated 0.5 hr. at 99°, acetylated, and chromatographed gave 580.9 mg. XI. XI (580 mg.) in 15 ml. C6H6 added in 20 min. to a Grignard agent from 3 g. MeI, 550 mg. Mg, and 15 ml. Et2O, stirred 1 hr., evaporated, refluxed 2 hrs. with 30 ml. C6H6, and the product acetylated gave 461.6 mg. dl-3α-acetoxy-17α-methyl-D-homo- androst-9(11)-en-17β-ol (XII), m. 184-6° (Me2CO-Et2O). XII (450 mg.) in 3.5 ml. C5H5N treated in the cold with 0.44 ml. POCl3, then heated 40 min. at 60-5°, the mixture treated with 380 mg. OsO4 in 0.46 ml. C5H5N and 15 ml. C6H6, and chromatographed on Al2O3 gave 110 mg. dl-3α-acetoxy-17α-methyl-D- homo-5β-androst-9(11)-ene-17β,17aβ-diol, m. 183-5° (Me2CO- Et2O), 67.8 mg. dl-3α-acetoxy-17β-methyl-D-homo-5β-androst-9(11)-ene-17α,17aα-diol (XIII), m. 181-3° (Me2CO-Et2O), 56.2 mg. dl-3α-acetoxy-17α-methyl-D-homo-5β-androst-9(11)-ene-16β,17β-diol (XIV), m. 205-7° (Me2CO-Et2O), and 48.3 mg. dl-3α-acetoxy-17β-methyl-D-homo-5β-androst-9(11)-ene-16α,- 17α-diol (XV), m. 196-7° (Me2CO-Et2O). dl-3α-Acetoxy-17β-methyl-D-homo-5β-androst-9(11)-ene-17β,17aβ-diol (100 mg.) in 3 ml. dioxane and 2.3 ml. MeOH left 2.5 hrs. at room temperature with 85 mg. HIO4·2H2O in 1.8 ml.

H2O gave 93.3 mg. dl-3α-acetoxy-16-acetyl-16,17-seco-5β-androst-9(11)-en-17-al (XVI), an oily residue. XIII (62 mg.) similarly treated with HIO4 gave 67 mg. XVI. Likewise, XIV and XV oxidized as above gave dl-3α-acetoxy-17-acetyl-16,17-seco-5β-androst-9(11)-en-16-al (XVII). XVI (160 mg.) in 4 ml. xylene heated 8 hrs. in a refluxing xylene bath in a sealed tube with 4 ml. xylene mixture prepared from 0.864 ml. AcOH and 1.4 ml. NEt3 in 10 ml. xylene and the product chromatographed on Al2O3 gave 76.8 mg. dl-3α-acetoxy-16-acetyl-5β-androsta-9(11),16-diene, m. 116-17° (Et2O-pentane). XVII (100 mg.) similarly treated gave 19.6 mg. dl-3α-acetoxy-5β-pregna-9(11),16-dien-20-one, m. 153-5° (MeOH or Et2O-pentane). Ir spectra were given for a number of the above described compds. I were useful in the synthesis of substances such as cortisone, hydrocortisone, prednisolone, and dexamethasone.

IT Steroids
(3-hydroxy 20-keto Δ9(11),16-)

IT Spectra, infrared
(of 3α-hydroxy-5β-pregna-9(11), 16-dien-20-one acetate and intermediates)

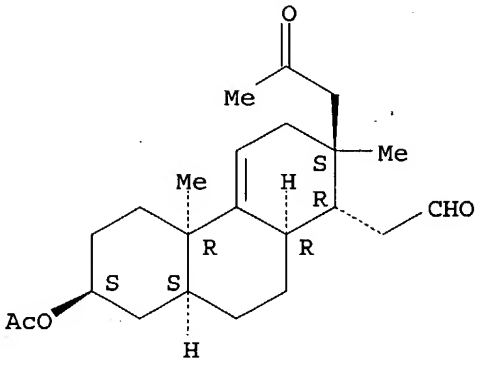
IT Spectra, visible and ultraviolet
(of 3α-hydroxy-5β-pregna-9(11),16-dien-20-one acetate and related compds.)

IT 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-, acetate
1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-, acetate
16,17-Seco-5β-androst-9(11)-en-17-al, 16-acetyl-3α-hydroxy-, acetate, (±)-
5β-Androsta-9(11),16-dien-3α-ol, 16-acetyl-, acetate, (±)-
5β-Pregna-9(11),16-dien-20-one, 3α-hydroxy-, acetate, (±)-
D-Homo-5α-androst-9(11)-ene-18-nitrile, 3α-hydroxy-17-oxo-, cyclic ethylene acetal, acetate, (±)-
D-Homo-5β-androst-9(11)-en-17-one, 3α-hydroxy-, acetate, (±)-
D-Homo-5β-androst-9(11)-en-17-one, 3α-hydroxy-, cyclic ethylene acetal, acetate, (±)-
D-Homo-5β-androst-9(11)-ene-18-nitrile, 3α-hydroxy-17-oxo-, acetate, (±)-
D-Homo-5β-gon-13(17a)-en-17-one, 3α-hydroxy-10-methyl-, (±)-
D-Homo-5β-gon-13(17a)-en-17-one, 3α-hydroxy-10-methyl-, (±)-, stereoisomer
D-Homo-5β-gon-13-en-17a-one, 3α-hydroxy-10-methyl-, acetate, (±)-
D-Homo-5β-gona-11,13(17a)-dien-17-one, 3α-hydroxy-10-methyl-, acetate, (±)-
D-Homo-5β-gona-12,17-diene-3α,17-diol, 10-methyl-, diacetate, (±)-
D-Homo-5β-gona-8,13,15,17-tetraen-3-one, 17-methoxy-10-methyl-, (±)-
D-Homo-5β-gona-8,13,15,17-tetraen-3α-ol, 17-methoxy-10-methyl-

IT 2574-60-9, D-Homo-5β-androst-9(11)-ene-3α,17β,17aβ-triol, 17-methyl-, 3-acetate, (±)- 2574-61-0, D-Homo-5β-androst-9(11)-ene-3α,17α,17aα-triol, 17-methyl-, 3-acetate, (±)- 2574-62-1, D-Homo-5β-androst-9(11)-ene-3α,16α,17α-triol, 17-methyl-, 3-acetate, (±)- 2574-63-2, D-Homo-5β-androst-9(11)-ene-3α,16β,17β-triol, 17-methyl-, 3-acetate, (±)- 2719-97-3, D-Homo-5β-androst-9(11)-ene-3α,17β-diol, 17-methyl-, 3-acetate, (±)- **2818-45-3**, 16,17-Seco-5β-pregn-9(11)-en-16-al, 3α-hydroxy-20-oxo-, acetate, (±)- 2887-17-4, Ketone, 3α-hydroxy-5β-androsta-9(11),16-dien-16-yl methyl, acetate, (±)- 4059-71-6, 2,4(1H,3H)-Quinazolinedione, 3-phenethyl- **97905-81-2**, 2-Phenanthrenecarboxaldehyde,

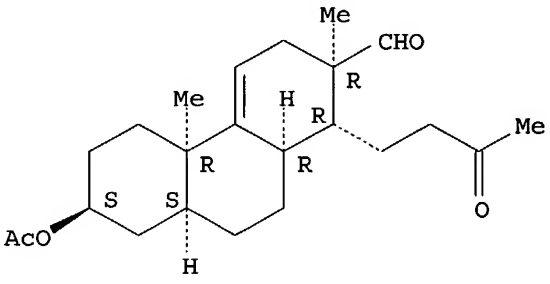
1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate
(preparation of)
IT 180-22-3, Spiro[chrysene-2(1H),2'-[1,3]dioxolane]
(steroid derivs.)
IT **2818-45-3**, 16,17-Seco-5β-pregn-9(11)-en-16-al, 3α-hydroxy-20-oxo-, acetate, (±)- **97905-81-2**, 2-Phenanthrenecarboxaldehyde, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate
(preparation of)
RN 2818-45-3 HCAPLUS
CN 16,17-Seco-5β-pregn-9(11)-en-16-al, 3α-hydroxy-20-oxo-, acetate, (±)- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 97905-81-2 HCAPLUS
CN 2-Phenanthrenecarboxaldehyde, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate (7CI) (CA INDEX NAME)

Relative stereochemistry.



L50 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1964:17095 HCAPLUS
DN 60:17095
OREF 60:3043h,3044a
ED Entered STN: 22 Apr 2001
TI 4-Chloro-3-oxo-Δ4-steroids
IN Tajima, Hiroaki; Yamada, Noji; Mori, Hiroshi
PA Teikoku Hormone Manufg. Co., Ltd.
SO 2 pp.
DT **Patent**
LA Unavailable
CC 42 (Steroids)
PATENT NO. KIND DATE APPLICATION NO. DATE

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 38018376		19630916	JP	19610215 <--

AB Into an agitated and cooled (0-5°) solution of 2 g. 17α-methyltestosterone acetate in 20 cc. pyridine is dropped 1 cc. sulfuryl chloride, the mixture agitated 1 hr., poured into 10% HCl, extracted with Et2O, the extract evaporated, and the residue recrystd. from Me2CO-hexane to give 1.8 g. 4-chloro-17α-methyltestosterone, m. 207-8°. Similarly prepared are 4-chloro-17α-acetoxyprogesterone (m. 179-82°) and 4-chloro-17α-ethynyltestosterone acetate (m. 196-8°). The compds. are useful as anabolic hormones.

IT Steroids
(4-chloro 3-keto Δ4-)

IT Spectra, visible and ultraviolet
(of 4-chloro 3-keto Δ4-steroids)

IT Steroids
(spirolactones)

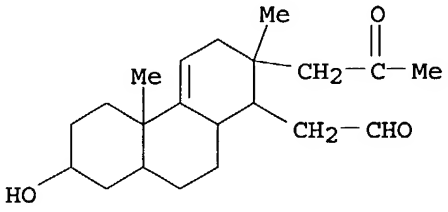
IT 20592-45-4, Pregn-4-ene-3,20-dione, 4-chloro-17-hydroxy-, acetate
96059-91-5, 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-
103937-32-2, 17α-Pregn-4-en-20-yn-3-one, 4-chloro-17-hydroxy-, acetate
(preparation of)

IT 180-22-3, Spiro[chrysene-2(1H),2'-[1,3]dioxolane] 317-06-6, Spiro[16H-cyclopenta[a]phenanthrene-16,2'(3'H)-furan]
(steroid derivs.)

IT **96059-91-5**, 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-
(preparation of)

RN 96059-91-5 HCAPLUS

CN 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl- (7CI) (CA INDEX NAME)



L50 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1964:17094 HCAPLUS

DN 60:17094

OREF 60:3043e-h

ED Entered STN: 22 Apr 2001

TI D-Homosteroid derivatives

IN Nagata, Wataru

PA Shionogi & Co., Ltd.

SO 9 pp.

DT **Patent**

LA Unavailable

CC 42 (Steroids)

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 38018374		19630916	JP	19600421 <--

AB A mixture (390 mg.) of 17-methyl-D-homoandrost-16-en-3β-ol 3-acetate and 17-methyl-D-homoandrost-17-en-3β-ol 3-acetate in 13 ml. C6H6 is kept at room temperature with 343 mg. OsO4 and 0.4 ml. pyridine 24 hrs., the

precipitate dissolved in 22 ml. dioxane, H2S gas passed in, the mixture filtered,
the filtrate evaporated, the residue extracted with CHCl3, and the extract evaporated and
chromatographed on Al2O3 to give: 13.2 mg. 17α-methyl-D-homoandrostane-3β,17β-17aβ-triol 3-acetate, m. 240-2° (Me2CO-Et2O-pentane); 39.1 mg. 17α-methyl-D-homoandrostane-3β,16β,17β-triol 3-acetate, m. 205-6°; 131.3 mg. 17β-methyl-D-homoandrostane-3β,17α, 17aα-triol 3-acetate, m. 203-4° and 206-7°, (double m.p.); and 98.1 mg. 17β-methyl-D-homoandrostane-3β,16α,17α-triol 3-acetate, m. 227-30°. Manufacture of the following are also described: 16,17-secopregnan-3β-ol-20-one-16-aldehyde 3-acetate (m. 112-15°), 16,17-seco-16-acetylandrostan-3β-ol-17-aldehyde 3-acetate (m. 118.5-20°), dl-16-acetylandrost-16-en-3β-ol 3-acetate (m. 163-5°), dl-pregn-16-en-3β-ol-20-one 3-acetate (m. 167-9°), 17α-methyl-D-homo-5β-androst-9(11)-ene-3α,17β-17aβ-triol 3-acetate (m. 154-6° and 183-5°; double m.p.), 17β-methyl-D-homo-5β-androst-9(11)-ene-3α, 17α,17aα-triol 3-acetate (m. 181-3°), 17α-methyl-D-homo-5β-androst-9(11)-ene-3α,16β,17β-triol 3-acetate (m. 205-7°), 17β-methyl-D-homo-5β-androst-9(11)-ene-3α,16α,17α-triol 3-acetate (m. 196-7°), 16-acetyl-16,17-seco-5β-androst-9(11)-ene-3α-ol-17-aldehyde 3-acetate (oil), 16,17-seco-5β-pregn-9(11)-en-3α-ol-20-one-16-aldehyde (oil), 16-acetyl-5β-androsta-9(11),16-dien-3α-ol 3-acetate (m. 116-17°), 5β-pregna-9(11),16-dien-3α-ol-20-one 3-acetate (m. 153-5°), D-homoandrost-5-ene-17ξ, 17aξ-diol-3,11-dione-18-nitrile 3-ethylene ketal (m. 240-61°), 17-formylandrosta-5,16-diene-3,11-dione-18-nitrile 3-ethylene ketal (m. 215-25°), and 16-formylandrosta-5,16-diene-3,11-dione-18-nitrile 3-ethylene ketal (m. 242-50°).

IT D-Homosteroids

IT Spectra, infrared
(of D-homosteroids)

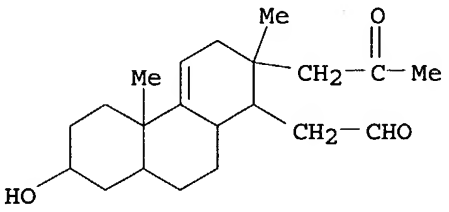
IT 5α-Androst-16-en-3β-ol, 16-acetyl-, acetate, (±)-
5α-Pregn-16-en-20-one, 3β-hydroxy-, acetate, (±)-
5β-Androsta-9(11),16-dien-3α-ol, 16-acetyl-, acetate
Ketone, 3β-hydroxy-5α-androst-16-en-16-yl methyl, acetate, (±)-
D-Homo-5α-androstane-3β,17β,17a;β-triol, 17-methyl-, 3-acetate
D-Homo-5β-androst-9(11)-ene-3α,17β,17aβ-triol, 17-methyl-, 3-acetate

IT 145-12-0, Androst-4-en-3-one, 4,17β-dihydroxy-17-methyl- 2747-16-2, Estr-4-en-3-one, 4,17β-dihydroxy-17-methyl- 3018-82-4, 5β-Pregna-9(11),16-dien-20-one, 3α-hydroxy-, acetate 13452-06-7, Androst-4-en-3-one, 4,17β-dihydroxy-, 17-acetate 68151-44-0, D-Homo-5α-androstane-3β,16α,17α-triol, 17-methyl-, 3-acetate 68151-46-2, D-Homo-5α-androstane-3β,16β,17β-triol, 17-methyl-, 3-acetate **96059-91-5**, 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl- 96464-87-8, 1-Phenanthreneacetaldehyde, 2-acetonyltetradecahydro-7-hydroxy-2,4b-dimethyl-, acetate 96464-88-9, 2-Phenanthrenecarboxaldehyde, tetradecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate **97905-81-2**, 2-Phenanthrenecarboxaldehyde, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate 100977-31-9, Gona-5,16-diene-16-carboxaldehyde, 13-cyano-10-methyl-3,11-dioxo-, cyclic 3-(ethylene acetal) 101296-52-0, 16,17-Seco-5α-androstan-17-al, 16-acetyl-3β-hydroxy-, acetate 101296-76-8, D-Homo-5β-androst-

9(11)-ene-3α,16β,17β-triol, 17-methyl-, 3 acetate
103071-38-1, D-Homo-5β-androst-9(11)-ene-3α,16α,17α-triol, 17-methyl-, 3-acetate 103424-11-9, Ketone, 3α-hydroxy-5β-androsta-9(11),16-dien-16-yl methyl, acetate 103536-44-3, D-Homo-5β-androst-9(11)-ene-3α,17α,17aβ-triol, 17-methyl-, 3-acetate 103937-18-4, D-Homoandrost-5-ene-18-nitrile, 17,17a-dihydroxy-3,11-dioxo-, cyclic 3-(ethylene acetal) 104073-44-1, Gona-5,16-diene-17-carboxaldehyde, 13-cyano-10-methyl-3,11-dioxo-, cyclic 3-(ethylene acetal)- 104836-58-0, D-Homo-5α-androstane-3β,17α,17aα-triol, 17-methyl-, 3-acetate
106423-85-2, 16,17-Seco-5β-pregn-9(11)-en-16-al, 3α-hydroxy-20-oxo- 106743-97-9, 16,17-Seco-5α-pregnan-16-al, 3β-hydroxy-20-oxo-, acetate
(preparation of)

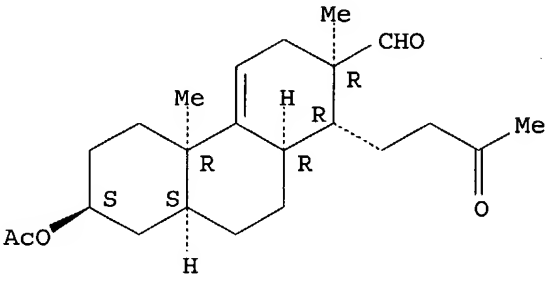
IT **96059-91-5**, 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-
97905-81-2, 2-Phenanthrenecarboxaldehyde, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate **106423-85-2**, 16,17-Seco-5β-pregn-9(11)-en-16-al, 3α-hydroxy-20-oxo-
(preparation of)

RN 96059-91-5 HCAPLUS
CN 1-Phenanthreneacetaldehyde, 2-acetonyl-1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl- (7CI) (CA INDEX NAME)



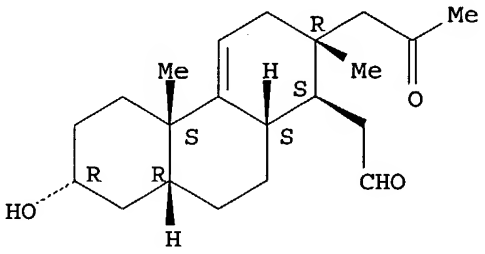
RN 97905-81-2 HCAPLUS
CN 2-Phenanthrenecarboxaldehyde, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-hydroxy-2,4b-dimethyl-1-(3-oxobutyl)-, acetate (7CI) (CA INDEX NAME)

Relative stereochemistry.



RN 106423-85-2 HCAPLUS
CN 16,17-Seco-5β-pregn-9(11)-en-16-al, 3α-hydroxy-20-oxo- (7CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1957:99387 HCAPLUS
DN 51:99387
OREF 51:18000g-i,18001a-b
ED Entered STN: 22 Apr 2001
TI 1,4b-Dimethyl-3-oxo-4a-hydroxy-7-isopropyltetradecahydrophenanthrene-1-carboxylic acid lactone
IN Sanderson, Thomas F.
PA Hercules Powder Co.
DT **Patent**
LA Unavailable
CC 10 (Organic Chemistry)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2785184		19570312	US	<--

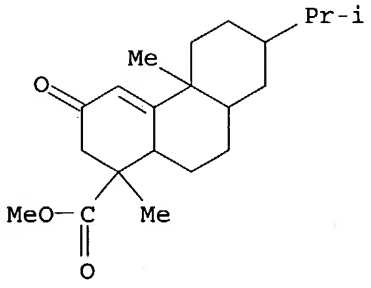
GI For diagram(s), see printed CA Issue.
AB I Me ester is prepared by refluxing I 30.4 in Me2CO 390 with addition of anhydrous K2CO3 13.8 followed by MeI 14.2 parts. The mixture was stirred and refluxed overnight; solids were removed by filtration. The filtrate was concentrated to 1/5 volume and diluted with 500 parts water. The mixture was extracted with ether, and the ether layer washed with water, dried over Na2SO4, and evaporated to dryness to give 30 parts I Me ester. The product treated with O in the presence of Co naphthenate absorbed in 3 hrs. at 90° 96 mole-% O. The mixture dissolved in ether, dried over Na2SO4, and evaporated to dryness gave 5.2 parts crystalline product, which showed λ 242 mμ, indicative of high α,β-unsatd. ketone content. The crystalline oxidate was dissolved in EtOH 24 containing Girard reagent 5 and AcOH 5 parts. The solution was refluxed 1 hr., cooled, diluted with ice water 100 containing NaOH 3, the mixture extracted 3 times with ether, and concentrated HCl 27 parts added to the aqueous layer. After standing 1 hr. the mixture was extracted with ether to yield α,β-unsatd. ketone 1.75 parts. The ketone was dissolved in diethylene glycol 23 containing KOH 1 part and the solution heated 1 hr. The solution was cooled, diluted with water, extracted with ether, the aqueous layer acidified, and the crystalline precipitate dissolved in ether to give IV, 167-8° (from MeOH).
IT 1-Phenanthrenecarboxylic acid, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-3-oxo-, (2,4-dinitrophenyl)hydrazone
IT 116-31-4, Retinal
(manufacture of)
IT **102707-59-5**, 1-Phenanthrenecarboxylic acid, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-3-oxo-, methyl ester 110248-19-6, 1-Phenanthrenecarboxylic acid, tetradecahydro-4a-hydroxy-7-isopropyl-1,4b-dimethyl-3-oxo-, γ-lactone **110662-55-0**, 1-Phenanthrenecarboxylic acid,

1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-, methyl ester
(preparation of)

IT **102707-59-5**, 1-Phenanthrenecarboxylic acid, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-3-oxo-, methyl ester **110662-55-0**, 1-Phenanthrenecarboxylic acid, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-, methyl ester
(preparation of)

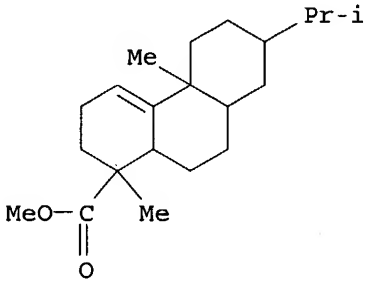
RN 102707-59-5 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-3-oxo-, methyl ester (6CI) (CA INDEX NAME)



RN 110662-55-0 HCAPLUS

CN 1-Phenanthrenecarboxylic acid, 1,2,3,4b,5,6,7,8,8a,9,10,10a-dodecahydro-7-isopropyl-1,4b-dimethyl-, methyl ester (6CI) (CA INDEX NAME)



L50 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1957:81769 HCAPLUS

DN 51:81769

OREF 51:14818f-i,14819a

ED Entered STN: 22 Apr 2001

TI Polycyclic ketones

PA C I B A Ltd.

DT **Patent**

LA Unavailable

CC 10 (Organic Chemistry)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	GB 768025		19570213	GB		<--

AB Δ1,9-2-Oxo-1-methyloctahydronaphthalenes treated with CH2:CHCOMe and alkaline reagents gives polycyclic ketones, which, when a tertiary HO group is present, can be dehydrated to form a compound with a double bond. To Δ1,9-2-oxo-1-methyloctahydronaphthalene (I) 10 in EtOH 30 stirred at 25° under N into NaOEt (from Na 1 in EtOH 100) and cooled to

-10° during 0.25 hr. is added CH2:CHCOMe 12 in EtOH 25 parts, the mixture stirred 16 hrs. at -5 to -10°, acidified with glacial AcOH, concentrated in vacuo, and extracted with ether, the extract washed with NaHCO3, dried with Na2SO4, and distilled, and the residue rectified in vacuo giving a mixture of stereoisomeric Δ5,13-11-hydroxy-2-oxo-12-methyldodecahydrophenanthrenes (II), b0.04 123-8°. One isomer seps. from the mixture in colorless lamellas, m. 135° (from n-hexane). II 43 in MeOH 680 treated in an N atmospheric with 10N NaOH 20, refluxed 1 hr., glacial AcOH 20 parts added, the MeOH distilled in vacuo, the residue extracted with ether, and the extract treated as above yields a mixture of stereoisomeric Δ1,11;5,13-2-oxo-12-methyldecahydrophenanthrene (III), yellow oil, b0.05 102-7°. The isomer of II, m. 135°, yields a crystalline isomer of III, m. 93°. III is also prepared by treating I with CH2:CHCOMe, NEt3, and NBu3 with or without pressure or with 4-piperidino-2-butanone under pressure. Similarly, Δ8,14-1,7-dioxo-8,11-dimethyldodecahydrophenanthrene is converted to Δ1,16;9,14-3,10-dioxo-13,17-dimethyl tetradecahydrochrysene (racemic Δ4;9,11-3,17a-dioxo-D-homoandrostadiene) (IV), m. 23-4° (from acetone). Chromatography over Carboraffin 50 and purified kieselguhr 100 parts and elution with acetone give an isomer of IV, m. 151.5-3.0°. Also, Δ8,14-1-ethylenedioxy-7-oxo-8,11-dimethyldodecahydrophenanthrene yields 2 isomers of Δ1,16;9,14-3-ethylenedioxy-10-oxo-13,17-dimethyltetradecahydrochrysene, m. 149-51° and 186-6.5° (from petr. ether or C6H6-petr. ether). These compds. are important for the manufacture of therapeutically useful steroids.

IT Steroids
(intermediates for)

IT Ketones
(polycyclic)

IT 1011-90-1, 1,3,6-Cycloheptatriene-1-acetamide, 6-hydroxy-5-oxo-
(Hofmann reaction of)

IT 533-75-5, Tropolone
(derivs.)

IT 169-43-7, Spiro[chrysene-1(2H),2'-[1,3]dioxolane]
(polyhydro derivs.)

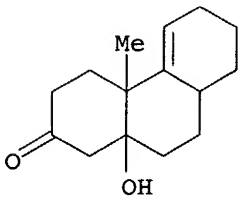
IT 74503-36-9, 2,2,3,3-Naphthalenetetracarbonitrile, 1,4,5,6,7,8-hexahydro-
98491-52-2, 2,4,6-Cycloheptatrien-1-one, 4-(aminomethyl)-2-hydroxy-
113011-63-5, D-Homoandrosta-4,9(11)-diene-3,17a-dione 124179-64-2,
D-Homoandrosta-4,9(11)-diene-3,17a-dione, cyclic 17a-(ethylene acetal)
(preparation of)

IT **108667-54-5**, 2(1H)-Phenanthrone, 3,4,4a,6,7,8,8a,9,10,10a-decahydro-10a-hydroxy-4a-methyl- 108979-96-0, 2(3H)-Phenanthrone, 4,4a,6,7,8,8a,9,10-octahydro-4a-methyl-
(stereoisomers)

IT **108667-54-5**, 2(1H)-Phenanthrone, 3,4,4a,6,7,8,8a,9,10,10a-decahydro-10a-hydroxy-4a-methyl-
(stereoisomers)

RN 108667-54-5 HCAPLUS

CN 2(1H)-Phenanthrone, 3,4,4a,6,7,8,8a,9,10,10a-decahydro-10a-hydroxy-4a-methyl- (6CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 13:16:11 ON 27 MAR 2004
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STRUCTURE FILE UPDATES:   26 MAR 2004  HIGHEST RN 668260-95-5
DICTIONARY FILE UPDATES:  26 MAR 2004  HIGHEST RN 668260-95-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> => d ide can tot

L52  ANSWER 1 OF 5  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   467222-38-4  REGISTRY
CN   1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-
     dodecahydro-1,4a,8-trimethyl-, methyl ester, (1R,4aR,8R,10aS)- (9CI)  (CA
     INDEX NAME)
FS   STEREOSEARCH
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SR   CA
LC   STN Files:   CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.  Rotation (-).
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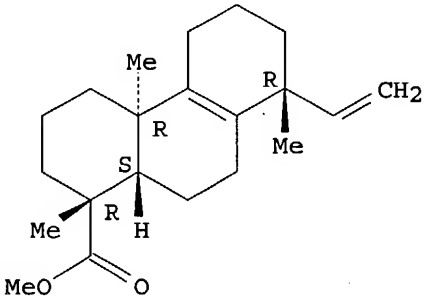

FYI - In applicants' references but excluded from search strategy

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORM

               3 REFERENCES IN FILE CA (1907
               3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1:  139:381626

REFERENCE   2:  138:238317
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REFERENCE 3: 137:279341

L52 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
RN **467222-37-3** REGISTRY
CN 1-Phenanthrenecarboxylic acid, 8-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,10aS)- (9CI) (CA INDEX NAME)
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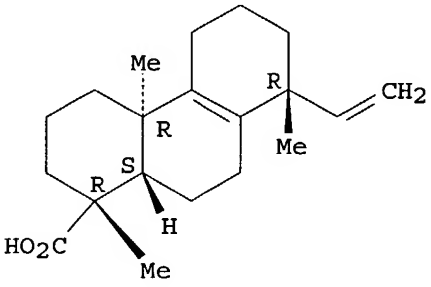
MF C20 H30 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

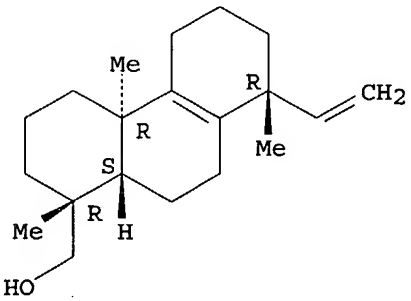
REFERENCE 1: 139:381626

REFERENCE 2: 138:238317

REFERENCE 3: 137:279341

L52 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
RN **467222-10-2** REGISTRY
CN 1-Phenanthrenemethanol, 8-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a,8-trimethyl-, (1R,4aR,8R,10aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H32 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

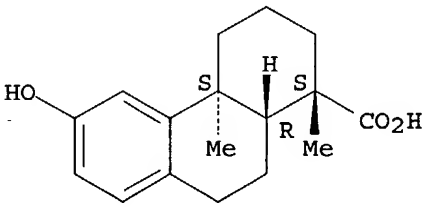
REFERENCE 1: 139:381626

REFERENCE 2: 138:238317

REFERENCE 3: 137:279341

L52 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
RN **5947-49-9** REGISTRY
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-6-hydroxy-1,4a-dimethyl-, (1S,4aS,10aR)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-6-hydroxy-1,4a-dimethyl-, [1S-(1α,4aα,10aβ)]-
CN Podocarpa-8,11,13-trien-16-oic acid, 12-hydroxy- (7CI, 8CI)
OTHER NAMES:
CN (+)-Podocarpic acid
CN (1S)-1,2,3,4,4a,9,10,10a-Octahydro-6-hydroxy-1,4a-dimethyl-1-phenanthrenecarboxylic acid
CN NSC 231784
CN Podocarpic acid
CN Podocarpic acid (C17H22O3)
FS STEREOSEARCH
MF C17 H22 O3
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, MEDLINE, MRCK*, NIOSHTIC, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

124 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
124 REFERENCES IN FILE CAPLUS (1907 TO DATE)
10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 139:381626

REFERENCE 2: 139:149390

REFERENCE 3: 139:69393

REFERENCE 4: 139:47197

REFERENCE 5: 138:51032

REFERENCE 6: 137:190040

REFERENCE 7: 135:235886

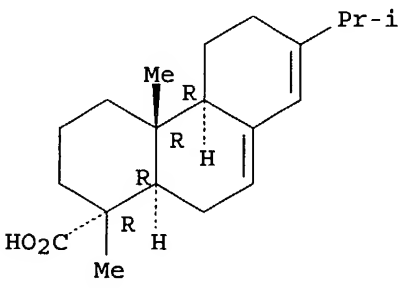
REFERENCE 8: 135:136542

REFERENCE 9: 135:41030

REFERENCE 10: 132:318113

L52 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
RN **514-10-3** REGISTRY
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R,4aR,4bR,10aR)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1α,4aβ,4bα,10aα)]-
CN Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- (8CI)
OTHER NAMES:
CN (-)-Abietic acid
CN 7,13-Abietadien-18-oic acid
CN Abietic acid
CN l-Abietic acid
CN NSC 25149
CN Odomit B 10
CN Sylvic acid
FS STEREOSEARCH
DR 72452-62-1
MF C20 H30 O2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2234 REFERENCES IN FILE CA (1907 TO DATE)

187 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2239 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 140:222603

REFERENCE 2: 140:201468

REFERENCE 3: 140:165575

REFERENCE 4: 140:129948

REFERENCE 5: 140:129197

REFERENCE 6: 140:113262

REFERENCE 7: 140:112687

REFERENCE 8: 140:110724

REFERENCE 9: 140:110722

REFERENCE 10: 140:98358

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